35th Annual Technical Meeting
Society of Engineering Science

SES'98

September 27-30, 1998

FINAL PROGRAM & BOOK OF ABSTRACTS

Edited by
Hussein M. Zbib

Washington State University
Pullman, Washington

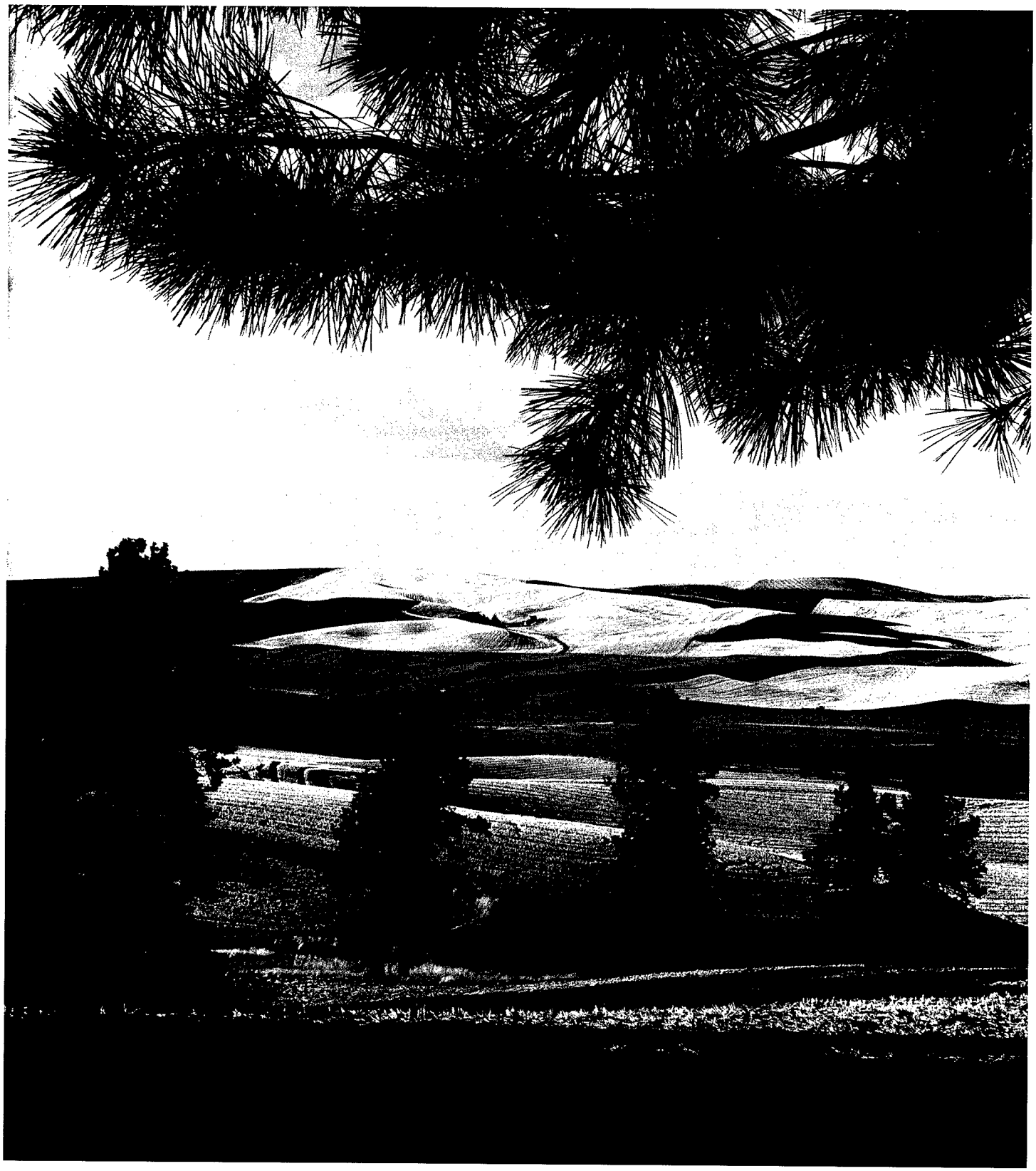
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14. ABSTRACT

The Society of Engineering Science (SES) 35th Technical Annual meeting was held on the campus of Washington State University in Pullman, Washington during the period Sept. 27-30, 1998. The main objective of the conference was to provide a forum for discussion and dissemination of recent advances in research, development and education, covering topics from all areas of engineering science. The SES98 consisted of 25 symposia composed of 110 sessions. A total of 510 technical papers were presented at these sessions including three plenary lectures. The central theme of the conference was "Engineering Science in the 21st Century: Bridging the Length Scales", addressing recent advances in engineering science, and identify long-term basic research issues and phenomena at various length scales (from atomic scale to continuum scale). Topics covered included, advances in fluids mechanics, solids mechanics, mechanics and materials, manufacturing, engineering physics, electrical engineering, biomechanics, soil mechanics, structural engineering, earthquake engineering, and nuclear engineering.

15. SUBJECT TERMS

solid mechanics, materials, fluid mechanics, biomechanics, electronic materials, fracture, plasticity, elasticity, dynamics.

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Society of Engineering Science 35th Annual Technical Meeting September 27 - 30, 1998 Washington State University Pullman, Washington

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We wish to acknowledge and thank all of those who have contributed to the meeting, including:

Sponsors

- **WSU School of Mechanical & Materials Engineering**
- **The Department of Mechanical Engineering at Texas Tech University**
- **WSU College of Engineering & Architecture**
- **Society of Engineering Science**
- **Pacific Northwest National Laboratory *(special thanks to Dr. Moe Khaleel)***
- **MARC Analysis Research Corporation *(special thanks to Dr. Reza Sadeghi)***
- **US Army Research Office, Engineering & Environmental Sciences Division *(special thanks to Dr. Kailasam Iyre and Dr. Mohamed Zikry)***
- **Office of Naval Research, Mechanics Division *(special thanks to Dr. Yapa Rajapakse)***
- **TexSEM Laboratories, Draper, UT**
- **NSF Industry Center for Design of Analog-Digital Integrated Circuits at WSU**
- **IEEE Electron Device Society, Pullman-Moscow Chapter**
- **The Boeing Company: Boeing Information, Space & Defense Systems**
- **Motorola Corporation**
- **Advanced Hardware Architectures, Pullman**
- **WSU Graduate & Professional Student Association**

Special Thanks:

- Special thanks to all the symposia organizers for the time and effort they volunteered towards inviting speakers, collecting and reviewing abstracts, and making this event a success.
- Special thanks to a number of people who spent countless number of hours during the whole process of the conference preparation, including:
  - ***Dr. Moe Khaleel** (PNL), for his continuous support and involvement throughout the lengthy process.
  - ***Typesetting**: Ms. Danielle Bishop and Ms. Barbara Williams
  - ***Conference Assistant**: Mr. Ahmed Younis.
  - ***Student Assistants:** *Mr. Tariq Khraishi, Mr. Moono Rhee, Ms. Meagan Taylor and Mr. Hassan Yasin*

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PLENARY SESSIONS

Plenary Session A1-1: Eringen Medal Symposium
Speaker: *Professor Pierre-Gilles de Gennes*
The 1998 Eringen Medal will be presented to Professor de Gennes. Professor de Gennes is a Nobel Laureate and won the award in Physics in 1991. He has made major contributions to the field of superconductivity, polymer physics, and magnetism. His books on liquid crystals and superconductivity are now classic. He is a member of the prestigious College de France and the French Academy of Sciences.

Plenary Session A2-1: Engineering Science Medal Symposium
Speaker: *Professor Sol Bodner*
Sol R. Bodner (M. S. from New York University, B.C.E. and Ph.D. from Polytechnic Institute of Brooklyn) has made notable contributions in modeling ballistic penetration /perforation and in the development of constitutive equations. He has also been active in the fields of dynamic plasticity of structures, wave propagation in solids, viscoelasticity, and composite materials. On these subjects he has authored and co-authored over 100 papers in the technical literature. He has served in both the academic world and as a consultant to the engineering industry, and is on the editorial advisory board of five engineering journals.

Plenary Session A3-1: Prager Medal Symposium
Speaker: *Professor J.R. Willis*
John R. Willis is Professor of Theoretical Solid Mechanics at the Department of Applied Mathematics and Theoretical Physics, University of Cambridge. He has been awarded numerous prizes for his outstanding research such as Lubbock Prize, University of London, 1961. Governors' Prize in Mathematics, Imperial College, London, 1961. Sherbrooke Research Studentship, University of London, 1961. Adams Prize, University of Cambridge, 1971. Timoshenko Medal from the Applied Mechanics Division of the ASME. He is an Elected Fellow, Institute of Mathematics and its Applications (FIMA), 1966, and Elected Fellow, Royal Society of London (FRS), 1992. He is the editor of the J, Mech. Phys. Solids (since 1982) and is member of editorial boards of: seven engineering journals. Professor Willis has made major contributions in Mathematical investigation of problems arising in the mechanics of solids, including the statics and dynamics of composite materials, dislocation theory (with recent application to strained-layer semiconductor devices), nonlinear fracture mechanics, elastodynamics of crack propagation, ultrasonic nondestructive evaluation.

Special Symposium to celebrate the 80th Birthday of ***Professor Edward W. Hart***
Edward W Hart is an emeritus Professor of Mechanics and Materials Science at Cornell University since 1976. Prior to that He served as a research scientist at GE for 25 years. He received his B.S. from the City University of New York in 1938. He worked as a Physicist and Electrical Engineer for the NAVY during World War II. He received the Meritorious Civilian Service Award for his work in the protection of NAVY ships against Magnetic Mines. Later he joined the graduate school of University of Berkeley and received his Ph.D. in 1950 in Nuclear Forces and Field Theory of Elementary Particles. After a brief Post-doctoral work, Dr. Hart joined General Electric Research Lab (now, Corporate Research and Development Center of GE Company). Professor Hart has been a pioneer in the dislocation theory of inelastic crystalline materials and developed many theories for dispersion hardening, dislocation dynamics, and grain boundary characterization. Most of his work in the last two decades has been in the formulation of Physically Based State Variable modeling of inelastic flow of Polycrystalline materials. His most recent contributions have been in the area Fracture Mechanics and crack propagation in an inelastic medium.

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Information on the conference is also available on the World Wide Web (www):
http://www.mme.wsu.edu/ses98.htm
http://www.eus.wsu.edu/c&i/programs/SES98.htm

SES'98
PROGRAM
September 27-30, 1998

Sunday September 27:

Reception and Registration (snack bar and refreshment)
5pm-9pm at the Lewis Alumni Center

Monday September 28:

Auditorium (CUB)

8:00am - 8:30am	Welcome
8:30am - 9:30am	**Plenary Session A1-1**
9:30am - 10:00am	Break/Poster Session / Refreshments

CUB Conference Meeting Rooms

10:00am - Noon	Technical Sessions I
Noon - 1:30pm	Lunch
1:30pm - 3:30pm	Technical Sessions II
3:30pm - 4:00pm	Break/Poster Session / Refreshments
4:00pm - 6:00pm	Technical Sessions III

Tuesday September 29:

Auditorium (CUB)

8:00am - 9:00am	**Plenary Session A2-1**
9:00am - 9:30am	Break/ Refreshments

CUB Conference Meeting Rooms

9:30am - 11:30am	Technical Sessions IV
11:30am- 1:00pm	Lunch
1:00pm - 3:00pm	Technical Sessions V
3:00pm-3:30pm	Break/Refreshments
3:30pm - 5:30pm	Technical Sessions VI

Banquet (CUB BALLROOM)

6:00pm - 7:00pm	Social Hour / Bar
7:00pm - 8:30pm	Dinner (Music)
8:30pm - 9:30pm	Program (Welcome, Awards, Music)

Wednesday, September 30:

Auditorium (CUB)

8:00am - 9:00am	**Plenary Session A3-1**
9:00am - 9:30am	Break/Refreshments

CUB Conference Meeting Rooms

9:30am - 11:30am	Technical Sessions VII
11:30am - 1:00pm	Lunch
1:00pm - 3:00pm	Technical Sessions VIII
3:00pm-3:30pm	Break/Refreshments
3:30pm - 5:30pm	Technical Sessions IX

Summary of Symposia and Session-Schedule

	Symposium and Organizer(s)	Sessions (Time Index)
A1	Eringen Medal Symposium. In honor of the Nobel Laureate Prof. Pierre-Gilles de Gennes. *A. C. Eringen*	A1-1 (M1), A1-2(M2), A1-3(M3), A1-4(M4) A1-5(T2), A1-6(T3), A1-7(T4) A1-8(W2)
A2	Engineering Science Medal Symposium: Constitutive Models and Penetration Mechanics. In honor of the 1998 Medalist Professor Sol Bodner. *K. S. Chan & C. Anderson (Southwest Research Institute)*	A2-1(T1), A2-2(M2), A2-3(M3), A2-4(M4)
A3	Prager Medal Symposium. In honor of the 1998 Prager Medalist Prof. John R. Willis. *P. P. Castaneda (U. of Pennsylvania)*	A3-1(W1), A3-2(T2), A3-3(T3), A3-4(T4) A3-5(W2), A3-6(W3), A3-7(W4)
B1	Numerical Modeling of Flow around Bluff Bodies. *S. Parameswaran (Texas Tech), A. Hadid (Boeing), V. Sumantran (GM), R. Sun (Chrysler) & S. S. Ravindran (NASA)*	B1-1(M2), B1-2(M3), B1-3(M4), B1-4(T4)
B2	Dynamics of Particles in Fluids in Dense Two-Phase Flows. *C. T. Crowe (WSU)*	B2-1(T2), B2-2(T3)
C1	Advanced Modeling in Geomechanics and Minerals Processing. *H. –B. Muhlhaus (CSIRO, Australia)*	C1-1(M2), C1-2(M3), C1-3(M4), C1-4(T2)
C2	Computational Methods for Granular Materials. *B. Loret (Inst. De Mech. De Grenoble) & M. Mehrabadi (Tulane U).*	C2-1(T3), C2-2(T4), C2-3(W2), C2-4(W3)
D1	Structural Dynamics, Nonlinear Dynamics and Control. *T. D. Burton & A. Barhorst (Texas Tech)*	D1-1(M2), D1-2(M3), D1-3(M4), D1-4(T2) D1-5(T3), D1-6(T4)
D2	Control Opportunities in Materials Processing. *J. Berg (Texas Tech)*	D2-1(T4), D2-2(W2), D2-3(W3), D2-4(W4)
E1	Mechanics, Micromechanics and Processing of Composites and Ceramics. *I. Demir (King Saud U), M. Garnich (PNL) & M. Khraisheh (King Fahd U)*	E1-1(T4), E1-2(W2), E1-3(W3)
E2	Compressive Failure in Fiber Composites. *A. Waas (Univ. of Mich.) & C. R. Schultheisz (NIST)*	E2-1(M2), E2-2(M3), E2-3(M4), E2-4(T2)
E3	Topics in Theoretical and Applied Elasticity. *Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)*	E3-1(M2), E3-2(M3), E3-3(M4), E3-4(T3) E3-5(T4), E3-6(W2), E3-7(W3)
E4	Mechanics and Materials Issues in Solid Polymers. *S. Ahzi (Clemson) & M. Negahban (Nebraska)*	E4-1(M2), E4-2(M3), E4-3(M4), E4-4(T2) E4-5(T3)
E5	Viscoelasticity in Composites. D. Allen (Texas A&M Univ.)	E5-1(T4), E5-2(W2)
F1	Inelastic Deformation and Failure. Symposium to celebrate Prof. E. Hart's 80th Birthday. *H. Garmestani (FSU) & F. G. Kollmann (Tech. Hochschule Darmstadt)*	F1-1(M2), F1-2(M3), F1-3(T2), F1-4(T3)
F2	Multi-Scale Modeling of Deformation and Fracture. *R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)*	F2-1(M2), F2-2(M3), F2-3(M4), F2-4(T2) F2-5(T3), F2-6(T4)
F3	Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. *M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)*	F3-1(M4), F3-2(T2), F3-3(T3), F3-4(T4) F3-5(W2), F3-6(W3), F3-7(W4)
F4	Failure Modes in Heterogeneous Materials. *M. Zikry (NCSU)*	F4-1(T4), F4-2(W2), F4-3(W3), F4-4(W4)
F5	Inelasticity and Material Instabilities. *D. Bammann (Sandia Nat'l Lab)*	F5-1(M2), F5-2(M3), F5-3(M4)
G1	Mechanics of Smart Structures. *H. Irschik (Joh. Kepler U, Austria)*	G1-1(M2), G1-2(M3), G1-3(M4), G1-4(T2)
G2	Phase Transformation in Active Materials. *A. Bhattacharyya (U. Alberta) D. Lagoudas (Texas A & M) & M. Taya (U. Washington)*	G2-1(T3), G2-2(T4), G2-3(W2), G2-4(W3) G2-5(W4)
H1	Giga Scale Integration Technology: Device, Process and IC Design. *M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)*	H1-1(M2), H1-2(M3), H1-3(M4), H1-4(T2) H1-5(T3)
H2	Mechanics and Sensing in Manufacturing Processes. *A. E. Bayoumi (NCSU)*	H2-1(T4), H2-2(W2), H2-3(W3), H2-4(W4)
I1	Biomechanics and Biomathematics. *K. Campbell (WSU) & C. Martin (Texas Tech)*	I1-1(T2), I1-2(T3)
P1	Poster Session	Throughout Monday

*See next page for Time Index , time and Room.

Total number of symposia: 25
Total number of sessions: 109
Total number of presentations: 475

SES'98 Session/Room Time-Table

Monday Sept. 28

Index	TIME	1. Auditorium (550)	2. Cascade 123 (100)	3. Cascade 125 (50)	4. Cascade 127 (70)	5. CUB 212 (80)	6. CUB 214-16 (30)	7. CUB 220 (40)	8. CUB 222 (30)	9. CUB 224 (30)	10. CUB 232 (30)	11. CUB B1-5 (50)	12. CUB B7-9 (30+)	13. CUB B11-15 (50)
M1	8:30a-9:30a	A1-1												
	9:30a-10:00a	**B R E A K / Poster Session/ Refreshments (Ballroom)**												
M2	10:00-12:00	D1-1	F2-1	E3-1	E2-1	G1-1	A2-2	A1-2	E4-1	F1-1	F5-1	H1-1	B1-1	C1-1
	12:00 - 1:30p	**L U N C H Buffet: (Ballroom)**												
M3	1:30p-3:30p	D1-2	F2-2	E3-2	E2-2	G1-2	A2-3	A1-3	E4-2	F1-2	F5-2	H1-2	B1-2	C1-2
	3:30p-4:00p	**B R E A K / Poster Session / Refreshments (Ballroom)**												
M4	4:00p-6:00p	D1-3	F2-3	E3-3	E2-3	G1-3	A2-4	A1-4	E4-3	F3-1	F5-3	H1-3	B1-3	C1-3

Tuesday Sept. 29

Index	TIME	1. Auditorium (550)	2. Cascade 123 (100)	3. Cascade 125 (50)	4. Cascade 127 (70)	5. CUB 212 (80)	6. CUB 214-16 (30)	7. CUB 220 (40)	8. CUB 222 (30)	9. CUB 224 (30)	10. CUB 232 (30)	11. CUB B1-5 (50)	12. CUB B7-9 (30+)	13. CUB B11-15 (50)
T1	8:00a-9:00a	A2-1												
	9:00a-9:30a	**B R E A K / Refreshments (Ballroom)**												
T2	9:30a-11:30	D1-4	F2-4	E2-4	A3-2	G1-4	I1-1	A1-5	E4-4	F3-2	F1-3	H1-4	B2-1	C1-4
	11:30a - 1:00p	**L U N C H Buffet: (Ballroom)**												
T3	1:00p-3:00p	D1-5	F2-5	E3-4	A3-3	G2-1	I1-2	A1-6	E4-5	F3-3	F1-4	H1-5	B2-2	C2-1
	3:00p-3:30p	**B R E A K / Refreshments (Ballroom)**												
T4	3:30p-5:30p	D1-6	F2-6	E3-5	A3-4	G2-2	H2-1	A1-7	E1-1	F3-4	F4-1	D2-1	B1-4	C2-2
												E5-1 in CUB 208		

Conference Banquet - 6-7pm : Social Hour. 7-10pm Dinner and Program

Wednesday Sept. 30

Index	TIME	1. Auditorium (550)	2. Cascade 123 (100)	3. Cascade 125 (50)	4. Cascade 127 (70)	5. CUB 212 (80)	6. CUB 214-16 (30)	7. CUB 220 (40)	8. CUB 222 (30)	9. CUB 224 (30)	10. CUB 232 (30)	11. CUB B1-5 (50)	12. CUB B7-9 (30+)	13. CUB B11-15 (50)
W1	8:00a-9:00a	A3-1												
	9:00a-9:30a	**B R E A K / Refreshments (Ballroom)**												
W2	9:30a-11:30	D2-2		E3-6	A3-5	G2-3	H2-2	A1-8	E1-2	F3-5	F4-2	E5-2		C2-3
	11:30a – 1:00p	**L U N C H Buffet: (Ballroom)**												
W3	1:00p-3:00p	D2-3		E3-7	A3-6	G2-4	H2-3		E1-3	F3-6	F4-3			C2-4
	3:00p-3:30p	**B R E A K / Refreshments (Ballroom)**												
W4	3:30p-5:30p	D2-4			A3-7	G2-5	H2-4			F3-7	F4-4			

***Speaker preparation room: CUB 208**

Monday Sept. 28

Monday Morning: 8:00am-8:30am
Welcome to WSU and SES'98
Auditorium

Monday Morning: 8:30am-9:30am
PLENARY SESSION A1-1

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel Laureate ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-1 Room: Auditorium, **Time:** M8:30a-9:30a
Chair: *T. Chang (MIT)*

8:30a-9:30a	Tentative Reflections on Powder Mechanics *Pierre-Gilles de Gennes*

9:30am-10:00am Poster session begins – Refreshments. Ballroom

Technical Sessions I
Monday Morning: 10:00am-12:00pm

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel Laureate ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-2 Room: CUB 220 **Time:** M10:00a-12:00p
Chair: *E. Samulski (U North Carolina)*

10:00a-10:24a	A Continuum Theory for Polymeric Liquid Crystals *A. C. Eringen*
10:24-10:48a	Twisting Constraints in Conventional Polymers *J. Plewa & T.A. Witten*
10:48a 11:12a	Structure and Dynamics of Block Copolymer Liquids *T. Lodge*
11:12a 11:36a	Measures of Integration in the Statistical Mechanics of Polymers and Liquid Crystals *W. Helfrich*

Symposium & organizer(s): A2- Engineering Science Medal Symposium: Constitutive Models and Penetration Mechanics. In honor of the 1998 Medalist **Professor Sol Bodner**. ***K. S. Chan & C. Anderson (Southwest Research Institute)***
Session: A2-2 Room: CUB214-16 **Time:** M10:00a-12:00p
Chair: *C. Anderson (Southwest Research Institute)*

10:00a-10:24a	Viscoplasticity at Static and Dynamic Loading Rates *E. Krempl & T. L. Sham*
10:24a-10:48a	A Model for Predicting Grain Boundary Cracking in Multi-Grain Crystalline Viscoplastic Materials *D. H Allen, K. L. E. Helms & L. D. Hurtado*
10:48a-11:12a	Propensity for Spall Formation in Salt Storage Caverns Using a Creep and Fracture Analysis. *D. E. Munson*
11:12a-11:36a	Application of Isochronous Healing Curves to Predicting Damage Evolution in a Salt Structure *K. S. Chan, D. E. Munson & S. R. Bodner*

Symposium & organizer(s): B1- Numerical Modeling of Flow around Bluff Bodies. ***S. Parameswaran (Texas Tech), A. Hadid (Boeing), V. Sumantran (GM), R. Sun (Chrysler) & S. S. Ravindran (NASA)***
Session: B1-1 Room: CUB B7-9 **Time:** M10:00a-12:00p
Chairs: *A. Hadid (Boeing) & S. Parameswaran (Texas Tech).*

10:00a-10:24a	Turbulence Modeling, Validation and Technology Transfer *P. G. Huang*
10:24-10:48a	Les Simulation of Turbulent Obstacle Flow Using Eddy-Viscosity Type Subgrid Models *A. H. Hadid, M. M. Sindir & S. Parameswaran*
10:48a 11:12a	Complex Vortex Dynamics in Bluff-Body Wakes. *R. Mittal*
11:12a 11:36a	Influence of Turbulence Models on the Prediction of Vortex Shedding from a Bluff Body *R. I. Issa*
11:36a-12:00p	On Large Eddy Simulation of Flow Over a Cylinder *P. Moin*

Symposium & organizer(s): C1- Advanced Modeling in Geomechanics and Minerals Processing. ***H. –B. Mühlhaus (CSIRO, Australia)***
Session: C1-1 Room: CUB B11-15 **Time**: M10:00a-12:00p
Chair: *H. B. Mühlhaus (CSIRO)*

10:00a-10:48a	**Keynote Lecture:** Damage Diffusion in Uniaxial Compression of Rocks *I. Vardoulakis, E. Papamichos & M. Bassanou*
10:48a-11:12a	Advanced Constitutive Relations for Geomaterials and Applications *F. Darve & X. Roguiez*
11:12a-11:36a	Modelling Comminution Devices Using DEM. *P.W. Cleary*
11:36a-12:00p	Balance Equations for the Mechanics of Poly Disperse Granular Materials *H. B. Mühlhaus & P. Hornby*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-1 Room: Auditorium **Time:** M10:00a-12:00p
Chairs: *T. D. Burton & A. A. Barhorst (Texas Tech)*

10:00a-10:24a	Numerically Stable Computation of the Lyapunov Characteristic Exponents for Continuous Dynamical Systems *F. E. Udwadia, & H. F. von Bremen*
10:24a-10:48a	Analytical Criterion for Chaotic Dynamics in Flexible Spacecraft with Nonlinear Controller Damping and Nonautonomous Forcing *G. L. Gray, & A. P. Mazzoleni*
10:48a-11:12a	A Preliminary Study of the Application of Floquet Multipliers to Nonlinear System Identification *R. I. Zadoks*

Symposium & organizer(s): E2- Compressive Failure in Fiber Composites. ***A. Waas (Univ. of Mich.) & C. R. Schultheisz (NIST)***
Session: E2-1 Room: Cascade 127 **Time:** M10:00a-12:00p
Chairs: *A. Waas (U. Mich.) & C. R. Schultheisz (NIST)*

10:00a-10:48a	**Keynote Lecture:** A Critical Review of Concepts Used to Explain the Compressive Properties of Fibre Composites *M. R. Piggott*
10:48a-11:12a	Nonlinear Viscoelastic Effects in the Compressive Strength of Unidirectional Fiber Composites *R. A. Schapery*
11:12a-11:36a	Research in Composites for Marine Structures: ONR Perspectives *Y. D. S. Rajapakse*
11:36a-12:00p	

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-1 Room: Cascade 125 **Time:** M10:00a-12:00p
Chairs: *C. Ru (U. Alberta) & P. Schiavone (U. Alberta)*

10:00a-10:24a	Saint-Venant Decay Rates for an Isotropic Inhomogeneous Linearly Elastic Solid in Anti-Plane Shear *C. Horgan*
10:24a-10:48a	Saint-Venant's Problem for a Second-Order Elastic Pretwisted Bar Using Signorini's Perturbation Method *F. Dell'Isola & R. C. Batra*
10:48a-11:12a	The Net Interaction Force Between Two Skew Dislocations in an Elastically Anisotropic Half-Space *D. M. Barnett*
11:12a-11:36a	Integral Equation Methods in Plane-Strain Elasticity With Boundary Reinforcement *P. Schiavone & C. Q. Ru*
11:36a-12:00p	Isoperimetric Inequalities for the Stresses Due to Inhomogeneities *L. Wheeler*

Symposium: E4 – Mechanics and Materials Issues in Solid Polymers
S. Ahzi (Clemson) & M. Negahban (Nebraska)
Session: E4-1 Room: CUB 222 **Time:** M10:00a-12:00p
Chairs: *A. Wineman (U. Mich.) & A. Gusev(Inst. Polymers)*

10:00a-10:48a	**Keynote Lecture:** Toughness Jumps in Particle Modified Polymers. *A. S. Argon*
10:48a-11:12a	Micromechanics of Particle-Toughened Semi-Crystalline Polymers. *P. Tzika, U. Baumann, M. C. Boyce & D. M. Parks*
11:12a-11:36a	Microstructure, Mechanical Performance and Deformation Behavior of Thermally Aged Polypropylene *R. Gensler, C. J. G. Plummer & H-H. Kausch*
11:36a-12:00p	Effect of Structure Property Relationships on the Electrical Conductivity, Mechanical Strength, and Optical Properties of Electroactive Polyaniline *R.V. Gregory*

Symposium & organizer(s): F1- Inelastic Deformation and Failure. Symposium to celebrate Prof. E. Hart's 80th Birthday. ***H. Garmestani (FSU) & F. G. Kollmann (Tech. Hochschule Darmstadt)***
Session: F1-1 Room: CUB 224 **Time:** M10:00a-12:00p
Chairs: *F. G. Kollman (Tech. Hochschule Darmstadt) & John Cahn*

10:00a-10:24a	Stress Relaxation and Strain Aging in Intermetallic TiAl *H. Mecking, S. Willems & A. Bartels*
10:24a-10:48a	Application of Modern Time Integrators to Hart's Model *E. Kirchner & F. G. Kollmann*
10:48a-11:12a	Anisotropic Stress/Strain-Rate Relations *U. F. Kocks*
11:12a-11:36a	Flow Stress of FCC Polycrystals with Application to OFHC CU. *S. Nemat-Nasser*
11:36a-12:00p	Modeling the Development of Residual Stresses in High Strength Steel Arising From Plastic Deformation *P. Dawson & D. Boyce*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. ***R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)***
Session: F2-1 Room: Cascade 123 **Time**: M10:00a-12:00p
Chairs: *T. D. de La Rubia (LLNL) & S. J. Zhou (LANL)*

10:00a-10:24a	Atomistic Finite Deformation Simulations *M. F. Horstemeyer & M. I. Baskes*
10:24a-10:48a	Atomistic Simulations for Multiscale Modeling in bcc Metals *J. A. Moriarty, W. Xu, P. Söderlind, J. F. Belak, J. Zhu, & L. H. Yang*
10:48a-11:12a	Atomistic Simulation of Dislocation of Intersection Process – A Step to Bridge Approaches Across Length Scale *S. J. Zhou & D. L. Preston*
11:12a-11:36a	Molecular Dynamics Simulations of Dislocation-Defect Interactions and Microstructure Evolution in Irradiated Metals *T. D. de la Rubia, E.A. Alonso & V. Shastry*
11:36a-12:00p	Elastic Interactions of Defects on Crystal Surfaces *D. Kouris, A. Peralta, J. Knap & K. Sieradzki*

Symposium & organizer(s): F5- Inelasticity and Material Instabilities. ***D. Bammann (Sandia Nat'l Lab)***
Session: F5-1 Room: CUB 232 **Time:** M10:00a-12:00p
Chairs: *M. Lusk (CO School of Mines) & K.T. Ramesh (Johns Hopkins)*

10:00a-10:24a	On a Modulated Energy Function for Modeling Recrystallization and Grain-Growth *M. T. Lusk*
10:24a-10:48a	Damage Localization Emerging from Microdamage Accumulation *H. L. Li, Y. Gu & Y.L. Bai*
10:48a-11:12a	Modeling Adiabatic Temperature Changes using Internal State Variables *G. C. Johnson, M. L. Chiesa & D. J. Bammann*
11:12a-11:36a	An Experiment of Thermoplastic Shear Band for a High Carbon Low Alloy Steel *Y. Yugong, S. Letian & Z. Xi*
11:36a-12:00p	Influence of Crystal Structure on the Dynamic Behavior of Materials at High Temperatures *A. M. Lennon & K. T. Ramesh*

Symposium & organizer(s): G1- Mechanics of Smart Structures. ***H. Irschik (Joh. Kepler U, Austria)***
Session: G1-1 Room: CUB 212 **Time:** M10:00a-12:00p
Chair: *H. Irschik (Joh. Kepler U., Austria)*

10:00a-10:48a	**Keynote Lecture**: Smart Materials and the Design of Solid-State Actuators *J. Wallaschek*
10:48a-11:12a	Active Magnetic Stabilization of an Unsymmetric Rotor-Bearing System *W. Kurnik & P. M. Przybyowicz*
11:12a-11:36a	Thermo-Visco-Elastic Analysis of High-Frequency Vibrations of Thin Plates *M. C. Dokmeci & G. A. Altay*
11:36a-12:00p	Axisymmetric Dynamics of Composite Spherical Panels with Composite and Active Piezoelectric Stiffeners *V. Birman, S. Griffin, G Knowles, & J Murray*

Symposium & organizer(s): H1- Giga Scale Integration Technology: Device, Process and IC Design. ***M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)***
Session: H1-1 Room: CUB B1-5 **Time:** M10:00a-12:00p
Chair: *K. Mayaram (WSU)*

10:00a-10:30a	Low Power Image and Communication Chip Technologies (Invited) *J. M. Stork*
10:30a-11:00a	Low Power Mixed-Signal Silicon Systems: Applications, Architectures, Technologies and Design Tools (Invited) *K. Shenai*
11:00a-11:30a	Low Temperature MOS Microelectronics Opportunities and Challenges (Invited) *M. J. Deen*
11:30a-12:00p	Optimization of DRAM Sense Amplifiers for the Gigabit Era *S. Parke*

LUNCH - 12:00pm – 1:30pm

Technical Sessions II
Monday Afternoon: 1:30pm-3:30pm

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel Laureate ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-3 Room: CUB 220 **Time:** M1:30p-3:30p
Chair: *T. Witten (U Chicago)*

1:30p-1:54p	Dynamic Surface Tension and Kinetics of Surfactant Adsorption at Fluid Interfaces *D. Andelman, H. Diamant & G. Ariel*
1:54p-2:18p	Polymers and Liquid Crystals: The Parallel World of Computational Models *A. Windle*
2:18p-2:42p	Ordered Phases of Block Copolymers and Lipids *M. Schick*
2:42p-3:06p	TITLE TO BE PROVIDED *S. Chandrasekhar*
3:06p 3:30p	Similarities in Liquid Crystals and Entangled Polymers *E.T. Samulski*

Symposium & organizer(s): A2- Engineering Science Medal Symposium: Constitutive Models and Penetration Mechanics. In honor of the 1998 Medalist Professor Sol Bodner. ***K. S. Chan & C. Anderson (Southwest Research Institute)***
Session: A2-3 Room: CUB 214-16 **Time:** M1:30p-3:30p
Chair: *R. C. Batra (VPI)*

1:30p-1:54p	Shear Band Spacing in Dipolar Thermoviscoplastic Materials *R. C. Batra & L. Chen*
1:54p-2:18p	Penetration of 6061-T6511 Aluminum Targets by Ogive-Nose Steel Projectiles with Striking Velocities Between 0.5 and 3.0 Km/s *T.L. Warren, A.J. Piekutowski, M. J. Forrestal and K.L. Poormon*
2:18p-2:42p	Use of Bodner-Partom Constitutive Model to Describe High Strain Rate and Shock Response of Several Metals. *A. M. Rajendran*
2:42p-3:06p	On the Hydrodynamic Approximation for Long-Rod Penetration *C. E. Anderson, Jr., D. L. Orphal, R. R. Franzen & J. D. Walker*

Symposium & organizer(s): B1- Numerical Modeling of Flow around Bluff Bodies. ***S. Parameswaran (Texas Tech), A. Hadid (Boeing), V. Sumantran (GM), R. Sun (Chrysler) & S. S. Ravindran (NASA)***
Session: B1-2 Room: CUB B7-9 **Time:** M1:30p-3:30p
Chair: *V. Sumantran (GM)*

1:30p-1:54p	Flow Induced Noise From Ground Vehicles-Problems and Prospects of Numerical Simulation. *S. R. Ahmed*
1:54p-2:18p	An Analysis of Some Numerical Simulation Issues Related to Bluff Body Aeroacoustics *S. R. Chakravarthy*, S. Palaniswamy, O. Peroomian & U. C. Goldberg
2:18p-2:42p	Computation of Trailing Edge Noise Using Large Eddy Simulation *P. Moin & M. Wang*
2:42p-3:06p	Computational Aeroacoustic Analysis System Development *A. H. Hadid, W. Lin, E. Ascoli, A. Darian, M. Stewart, S. Barson & M. Sindir*
3:06p-3:30p	Model Equations for the Calculation of Deforming Surfaces in Non-Steady Flows *Z. U. A. Warsi*

Symposium & organizer(s): C1- Advanced Modeling in Geomechanics and Minerals Processing. ***H. –B. Muhlhaus (CSIRO, Australia)***
Session: C1-2 Room: CUB B11-15 **Time:** M1:30p-3:30p
Chairs: *L. J. Sluys (Delft) & F. Oka (Kyoto)*

1:30p-1:54p	A Gradient Field Theory: Nanomechanics of Self-Organization and Localization *K. C. Valanis*
1:54p-2:18p	Localization Analysis of Water-Saturated Cohesive Soil *F. Oka, A. Yashima & K. Sawada*
2:18p-2:42p	Shear Band Phenomena in Empty and Saturated Soils Computed by Time and Space-Adaptive Methods *W. Ehlers, P. Ellsiepen & W. Volk*
2:42p-3:06p	3D Adaptive Viscoplastic Modeling of Shear Banding *L. J. Sluys, W. M. Wang & H. Askes*
3:06p-3:30p	A Microstructure Model for Elastic Surface Effects and Spalling *E. Dawson*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-2 Room: Auditorium **Time:** M1:30p-3:30p
Chair: *T.D. Burton & A. A. Barhorst (Texas Tech)*

1:30p-1:54p	A Helicopter Individual Blade Control with a "Smart" Spring at the Root *A. Solaiman, F. Afagh & F. Nitzsche*
1:54p-2:18p	Dynamic Modeling and Experimental Verification of a Flexible-Follower Quick-Return Mechanism *S. King & A. A. Barhorst*
2:18p-2:42p	Modal Reduction of Some Non-Linear Finite Element Models Using High-Dimensional Invariant Manifolds. *E. Pesheck & C. Pierre*
2:42p-3:06p	Effect of Internal Resonance on Model Reduction in Nonlinear Structural Dynamics *T. D. Burton & W. Rhee*
3:06p-3:30p	Closed-Form Modeling of Fluid-Structure Interaction – Navier-Stokes Case *J. L. Ortiz*

Symposium & organizer(s): E2- Compressive Failure in Fiber Composites. ***A. Waas (Univ. of Mich.) & C. R. Schultheisz (NIST)***
Session: E2-2 Room: Cascade 127 **Time:** M1:30p-3:30p
Chairs: *Y. Rajapakse (ONR) & R.A. Schapery (U. Texas-Austin)*

1:30p-1:54p	Dynamic Compressive Behavior of Glass Fiber Reinforced Unidirectional Vinyl Ester Composites. *A. M. Waas, S. H. Lee, N. Takeda & J. M. Yuan*
1:54p-2:18p	Mixed-Mode Stress Intensity Factors for Composite Plates with Single Delamination Under Compression *H. Huang & G. A. Kardomateas*
2:18p-2:42p	On the Determination of Strain Energy Release Rates in 2-Dimensional Delamination Buckling Scenarios *M. J. Johnson & S. Sridharan*
2:42p-3:06p	Failure of Laminated Composites at Thickness Discontinuities Under Complex Loading and Elevated Temperatures *S. Lee & W. G. Knauss*
3:06p-3:30p	Buckling Simulations of Composite Sandwich Panels with Core to Face Delaminations *E. Riks & C. C. Rankin*

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-2 Room: Cascade 125 **Time:** M1:30p-3:30p
Chair: *P. Rosakis (Cornell)*

1:30p-1:54p	Fluid Capillarity with Curvature-Dependent Elasticity. *D. Steigmann*
1:54p-2:18p	A Simple, Logical, Comprehensive Approach to Nonlinear Shell Theory *J. G. Simmonds*
2:18p-2:42p	Extensional Oscillations and Waves in Elastic Rods Which Account for Thickness-Stretch Effects *S. Krishnaswamy*
2:42p-3:06p	Extremum Principles for Nonlinearly Elastic Membrane Problems *R. W. Ogden & J. B. Haddow*
3:06p-3:30p	On Calculation of Interfacial Stresses in Film-Substrate Systems. *C. Ru*

Symposium: E4 –Mechanics and Materials Issues in Solid Polymers
S. Ahzi (Clemson) & M. Negahban (Nebraska)
Session: E4-2 Room: CUB 222 **Time:** M1:30p-3:30p
Chairs: *E. Arruda (U. Mich.) & R Seguela (U. Sci & Tech)*

1:30p-1:54p	Time Dependent Viscosity and Physical Aging in Polymers and Polymer Composites S.F. Zheng & *G.J. Weng*
1:54p-2:18p	Modeling of the Competition Between Shear Yielding and Brittle Failure by Crazing in Amorphous Polymers *R. Estevez & E. Van der Giessen*
2:18p-2:42p	Modeling Mechanical, Thermal, and Electric Properties of Composite Materials *A. A. Gusev*
2:42p-3:06p	Modeling of the Elastic-Inelastic Response of Layered SL5170 Resin Parts Produced by Stereolithography *S. Ahzi*
3:06p-3:30p	Predicting Local Damage in Unidirectional Composites *M. Rozman & A. A. Gusev*

Symposium & organizer(s): F1- Inelastic Deformation and Failure. Symposium to celebrate Prof. E. Hart's 80th Birthday. ***H. Garmestani (FSU) & F. G. Kollmann (Tech. Hochschule Darmstadt)***
Session: F1-2 Room: CUB 224 **Time:** M1:30p-3:30p
Chairs: *John Hirth (WSU) & R. Thompson (NIST)*

1:30p-1:54p	Crack Arrest in Silicon Single Crystals Leading to Brittle-to-Ductile Transitions in Fracture. *A. S. Argon & B. Gally*
1:54p-2:18p	Internal Variable Theory Revisited: Gradient and Stochastic Effects. *E. C. Aifantis*
2:18p-2:42p	Use of Nonproportional and Sequence Experiments to Study the Structure of ISV Constitutive Relations. *D. L. McDowell*
2:42p-3:06p	Ultra-Small-Angle X-Ray Scattering by Single Crystal Al Deformed In-Situ *L. E. Levine, G. G. Long & R. Thomson*
3:06p-3:30p	Consideration of Processes on the Microscale and Mesoscale for the Development of Constitutive Models for Metallic Materials *E. A. Steck*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. ***R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)***
Session: F2-2 Room: Cascade 123 **Time:** M1:30p-3:30p
Chairs: *N. M. Ghoniem (UCLA) & H. Huang (LLNL)*

1:30p-1:54p	Interaction Between Curved Dislocation Segments in 3-D Dislocation Dynamics *N. M. Ghoniem & M. Baccaloni*
1:54p-2:18p	Study of Frank-Read Sources Within a Continuum Simulation. *D. C. Chrzan*
2:18p-2:42p	Dislocation Dynamics from Kröner to Simulation and a Proposed New Dynamical Treatment. *A. A. El-Azab*
2:42p-3:06p	Stability of Dislocation Short-Range Reactions in BCC Crystals *H. Huang, N. Ghoniem, T. D. de la Rubia, M. Rhee, H. M. Zbib & J. P. Hirth*
3:06p-3:30p	3D Dislocation Dynamics: Treatment of Long and Short Range Interactions. *M. Rhee, H. M. Zbib, J. P. Hirth, T. de la Rubia & H. Huang.*

Symposium & organizer(s): F5- Inelasticity and Material Instabilities. ***D. Bammann (Sandia Nat'l Lab)***
Session: F5-2 Room: CUB 232 **Time:** M1:30p-3:30p
Chairs: *D. Bammann (Sandia) & D. A. Hughes (Sandia)*

1:30p-1:54p	Quantitative Representations of Dislocation Patterns from Experiments *D. A. Hughes & A. Godfrey*
1:54p-2:18p	Use of the Weibull Distribution to Model Variations in Ceramic DOP Results *N. L. Rupert & F. I. Grace*
2:18p-2:42p	The Influence of Gradient Terms in the Evolution Equations on Dislocation Density Distributions *D. Bammann & P. Dawson*
2:42p-3:06p	Full Field Measurements of Shear Dominated Fracture in Dynamic Two Dimensional Punch Tests on High-Strength Metals *K. M. Roessig & J. J. Mason*
3:06p-3:30p	An Energy-Based Approach for Modeling Inelasticity *G. Grach, M. T. Lusk & D. Bammann*

Symposium & organizer(s): G1- Mechanics of Smart Structures. ***H. Irschik (Joh. Kepler U., Austria)***
Session: G1-2 Room: CUB 212 **Time:** M1:30p-3:30p
Chair: *M. Krommer & H. Irschik (Joh. Kepler U. Austria)*

1:30p-1:54p	Thermodynamic Derivation of Dynamic Boundary Value Problem and Heat Conduction Equation for Piezothermoelastic Materials. *A. K. Belyaev*
1:54p-2:18p	A Reissner-Mindlin-Type Plate Theory Including the Direct Piezoelectric and the Pyroelectric Effect *H. Irschik & M. Krommer*
2:18p-2:42p	Piezoelectric Vibrations of Composite Beams with Interlayer Slip *R. Heuer & C. Adam*
2:42p-3:06p	Optimal Control of Plate Vibrations by Piezoelectric Sensors and Actuators *A. Kugi, K. Schlacher & H. Irschik*
3:06p-3:30p	Transient Response of a Cracked Piezoelectric Strip Under Arbitrary Anti-Plane Impact *S. W. Yu & Z.T. Chen*

Symposium & organizer(s): H1- Giga Scale Integration Technology: Device, Process and IC Design. ***M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)***
Session: H1-2 Room: CUB B1-5 **Time:** M1:30p-3:30p
Chair: *M.A. Osman (WSU)*

1:30p-2:00p	Predictive Models for Semiconductor Device Design and Processing (Invited) *M. Meyyappan*
2:00p-2:30p	Simulation Needs for Ultra-Scaled Silicon Devices (Invited) *U. Ravaioli*
2:30p-3:00p	Statistical Modeling From Case Files and Process Monitoring Data *K. Singhal & V. Fisvanathan*
3:00p-3:30p	Simulation of Ultra-Small MOSFETs Using a 2-D Quantum-Corrected Drift-Diffusion Model *B. A. Biegel, C. S. Rafferty, Z. Yu, M. G. Ancona & R. W. Dutton*

3:30pm-4:00pm Poster session – Refreshments. Ballroom

Poster Session

Session: P1-1 Room: CUB Ballroom **Time:** All Day Monday

Analytical Determination of Cyclic Hydrostatic Stress-Strain Relations for a Composite Sphere with a Soft Inclusion and a Hard Bilinear, Isotropically Hardening Matrix
E.J. Appiah and A. Bhattacharyya

Air Flow and Exhaust Dilution Rates From Johnson Hall Wind Tunnel Study
L. Gu & Z. Zanol

Different Methods to Determine the Surface Areas of Polar Molecules Absorbed on Solid Surfaces
T. Hamieh

A New Method to Calculate the Surface Potential of an Air Bubble Moving an Inclined Surface
T. Hamieh and D. Li

Modeling of Dynamic Failure in a Wide Range of Temperature and Pressure
S. Hanim and S. Ahzi

Time-Dependent Subloading Surface Model for Soils
K. Hashiguchi

A Parametric Study of Void Growth in Superplastic Deformation
T.A. Khraishi, M. Khaleel, H.M. Zbib

Study of Forced Convection Boiling in Microgravity
Y. Ma

Effects of Self-Heating on Gate Transconductance (g_m) of Silicon-On-Insulator MOSFETS
A.A. Osman and M.A. Osman

Moisture Effects on Strength Parameters of a Wood-Thermoplastic Composite Material
S.V. Rangaraj and L.V. Smith

Second-order Estimates for the Effective Behavior of Particle-Reinforced Rubbers
E. Tiberio

Fatigue and Damage Accumulation
G. Wheatley

A Numerical Study of Conjugate Gradient Directions for an Ultrasound Imaging Application
X. Zhang and S.L. Broschat

Effects of Particle Interaction and Size Variation on Damage Evolution in Filled Elastomers
X.A. Zhong and W.G. Knauss

Technical Sessions III
Monday Afternoon: 4:00pm-6:00pm

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel *Laureate* ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-4 Room: CUB 220 Time: M4:00p-6:00p
Chair: *D. Andelman (Tel Aviv U)*

4:00p-4:24p	Using Stochastic Simulations to Study the Dynamics of Polymer Melts and Liquid Crystals *J. Schieber*
4:24p-4:48p	Polymers, Liquid Crystals and Molecular Shuttles *J.R. Dennis, J. Howard & V. Vogel*
4:48p-5:12p	Smectic a Liquid Crystals as Modulated Nematics: Phase Transition Studies *C. Calderer*
5:12p-5:36p	Liquid Crystals and the Physics of Defects *M. Kleman*
5:36p 6:00p	Chiral Mesophases of DNA *R.D. Kamien*

Symposium & organizer(s): A2- Engineering Science Medal Symposium: Constitutive Models and Penetration Mechanics. In honor of the 1998 Medalist Professor Sol Bodner. ***K.S. Chan & C. Anderson (Southwest Research Institute)***
Session: A2-4 Room: CUB 214-16 **Time**: M4:00p-6:00p
Chair: *K. S. Chan (Southwest Research Institute)*

4:00p-4:24p	Fracture of Yawed Rods that Penetrate Finite Plates. *S. J. Bless & S. Satapathy*
4:24p-4:48p	Response Sensitivities, Parameter Estimation, and the Bodner-Partom Equations. *A. F. Fossum & P. E. Senseny*
4:48p-5:12p	Nontraditional Striker Impact. *W. Goldsmith*
5:12p-5:36p	Techniques for Measurement and Constitutive Modeling of Dynamic Deformation *A. S. Khan*

Symposium & organizer(s): B1- Numerical Modeling of Flow around Bluff Bodies. ***S. Parameswaran (Texas Tech), A. Hadid (Boeing), V. Sumantran (GM), R. Sun (Chrysler) & S. S. Ravindran (NASA)***
Session: B1-3 Room: CUB B7-9 **Time:** M4:00p-6:00p
Chair: *S. S. Ravindran (NASA)*

4:00p-4:24p	Advances in Optimal Control of Navier-Stokes Equation *S. S. Sritharan*
4:24p-4:48p	Adaptive Shape Sensitivity Calculations in Thermal Fluids *J. Borggarrd*
4:48p-5:12p	Active Flow Control *N. Chokani*
5:12p-5:36p	Optimal and Robust Reduced-Order Feedback Control of Turbulent Channel Flows *L. Cortelezzi, J. L. Speyer, K-H. Lee & J. Kim*

Symposium & organizer(s): C1- Advanced Modeling in Geomechanics and Minerals Processing. **H. –B. Muhlhaus (CSIRO, Australia)**
Session: C1-3 Room: CUB B11-15 **Time**: M4:00p-6:00p
Chairs: *E. Dawson (Dames & Moore) & H. Horii (U. of Tokyo)*

4:00p-4:24p	Lagrangian Particle Modelling of Silo Flows *L. Moresi & H.B. Muhlhaus*
4:24p-4:48p	Micromechanics-Based Continuum Modeling for Solids with Discontinuities. *H. Horii*
4:48p-5:12p	Anisotropic Hardening of Fiber-Reinforced Granular Composites *R. L. Michalowski*
5:12p-5:36p	Micro-Structure Developed in Shear Bands and Its Implication in the Mechanics of Granular Media *M. Oda & K. Iwashita*
5:36p-6:00p	Localization Analysis by the Subloading Surface Model with a Tangential Stress Rate Effect. *K. Hashiguchi*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-3 Room: Auditorium **Time:** M4:00p-6:00p
Chair: *F. E. Udwadia (U. Southern California)*

4:00p-4:24p	Design of Adaptive Sliding Mode Controller for Robot Manipulators *A. M. Aledhaibi, B. H. Lu & J-K. Huang*
4:24p-4:48p	Time Delayed Control of Classically Damped and Non-Classically Damped Structural Systems. *F. E. Udwadia, H. F. von. Bremen & M. Wilson*
4:48p-5:12p	Sliding Mode Control-Dynamic Observer for a Slewing Flexible Link *D. G. Wilson, G. G. Parker, G. P. Starr & R. D. Robinett*
5:12p-5:36p	Vibration Control of an Elastic Shaft and Elastic Link Manipulator *A. A. Ankarali, Z. Mecitolu, & H. Diken*
5:36p-6:00p	Vibrational Method in Order to Value the Damage Caused by Unfit Lubrication of the Ball Bearings *F. Blosio , M. Cavacece & C. Luvidi*

Symposium & organizer(s): E2- Compressive Failure in Fiber Composites. ***A. Waas (Univ. of Mich.) & C. R. Schultheisz (NIST)***
Session: E2-3 Room: Cascade 127 **Time:** M4:00p-6:00p
Chairs: *W. S. Slaughter (U. Pittsburgh) & G. Ravichandran (Cal. Inst. Tech)*

4:00p-4:24p	Buckling and Failure of Axially-Loaded Elliptical Composite Cylinders *M. W. Hyer & C. A. Meyers*
4:24p-4:48p	Prediction of Compressive Strength of Multi-Directional Composites. *J. Y. Shu*
4:48p-5:12p	Compression Failure in Graphite Epoxy Composites by Kink Band Formation: A Study Based on Random Breaks Causing Kink Band Initiation *S. Narayanan & L. S. Schadler*
5:12p-5:36p	A Model for Through-the-Thickness Effects in Compression Failure of Fiber Composites *S. R. Swanson*
5:36p-6:00p	A Geometrically Nonlinear Analysis of Compressively Loaded Prismatic Plate Structures Using a Reduced Basis Method *S. A. Ragon & Z. Gürdal*

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-3 Room: Cascade 125 **Time:** M4:00p-6:00p
Chair: *S. Krishnaswamy (Nebraska-Lincoln)*

4:00p-4:24p	Natural Strain Invariants for Isotropic Finite Hyperelasticity. *J. C. Criscione, J. D. Humphrey & W. C. Hunter*
4:24p-4:48p	On the Existence of a Stretch for a Prescribed Stress in Isotropic, Incompressible Elastic Materials. *T. R. Nordenholz & O. M. O'Reilly*
4:48p-5:12p	The Inverse Convexity Condition and Its Implications in Nonlinear Elasticity. *P. Rosakis*
5:12p-5:36p	New Existence Results in Nonlinear Elastostatics via Global Continuation Methods *T. Healey*
5:36p-6:00p	On the Application of Covariance to Anisotropic Finite Elasticity *P. Papadopoulos & J. Lu*

Symposium: E4 –Mechanics and Materials Issues in Solid Polymers
S. Ahzi (Clemson) & M. Negahban (Nebraska)
Session: E4-3 Room: CUB 222 **Time:** M4:00p-6:00p
Chairs: *M. Negahban (U. Nebraska) & M. E. Godard (U. De Rouen, France)*

4:00p-4:24p	Time Dependent Deformation in Elastomeric Materials. *J. Bergstrom & M. C. Boyce*
4:24p-4:48p	Structure-Property Relationship In Glassy Polymers Through the Tool-Moynihan-Narayanaswamy Relationship *M-E. Godard & J-M. Saiter*
4:48p-5:12p	Biaxial, Nonlinear Behavior of Solid Polymers. *H-B. Lu & C. V. Velvadapu*
5:12p-5:36p	Monte Carlo Modeling of Polymer Deformation. *C. Chui & M. C. Boyce*
5:36p-6:00p	AFM Observation of Microscopic Behavior of Glassy Polymer and Constitutive Modellings *Y. Tomita, T. Adachi, and S. Tanaka*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. ***R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)***
Session: F2-3 Room: Cascade 123 **Time:** M4:00p-6:00p
Chairs: *D. Lassila (LLNL) & W. King (LLNL)*

4:00p-4:24p	Time-Resolved Response of Shocked Materials at Different Length Scales. *Y. Gupta*
4:24p-4:48p	Experimental Investigation of Size Effects of FCC Polycrystal by Shear Banding *O. Watanabe & T. Kurata*
4:48p-5:12p	Experimental Study of Internal Variable Evolution in 304L Stainless Steel at Multiple Strain Rates and Temperatures *E. J. Harley, M. P. Miller, & D. J. Bammann*
5:12p-5:36p	Mechanical Behavior of Ta and Ta-W Alloys and Their Associated Dislocation Structures *C.L. Briant, C. Bull, & D.H. Lassila*
5:36p-6:00p	Orientation Imaging Microscopy Investigation of the Compression Deformation of A [110] Ta Single Crystal *A. J. Schwartz, W. E. King, G. H. Campbell, D. H. Lassila, D. Sam & J.Y. Shu*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-1 Room: CUB 224 **Time:** M4:00p-6:00p
Chairs: *T. R. McNelley (Naval Postgraduate School) & T. Bieler (Mich. State U.)*

4:00p-4:24p	Initiation and Early Stages of Cavity Growth During Superplastic and Hot Deformation *A. K. Ghosh, D-H Bae & S.L. Semiatin*
4:24p-4:48p	Characterization of Grain Boundary Evolution during Processing and Deformation of Superplastic Aluminum Alloys *T. R. McNelley*
4:48p-5:12p	A Mechanism for Deformation-Enhanced Grain Growth during Superplastic Deformation. *C. H. Hamilton*
5:12p-5:36p	Role of Local Composition on Interfacial Sliding *J. S. Vetrano, C. H. Henager, Jr. & S. M. Bruemmer*
5:36p-6:00p	The Effect of Threshold Stresses on High Strain Rate Superplastic Formability when Thermal and Strain Rate Gradients Exist *T. R. Bieler*

Symposium & organizer(s): F5- Inelasticity and Material Instabilities. ***D. Bammann (Sandia Nat'l Lab)***
Session: F5-3 Room: CUB 232 **Time:** M4:00p-6:00p
Chairs: *H. Zahrounii (U. of Metz) & A. D. Gupta (US-ARL)*

4:00p-4:24p	Micromechanics based on the Non-Riemannian Plasticity *T. Hasebe & Y. Imaida*
4:24p-4:48p	Modeling and Analysis of an Asymmetric Mine-Soil-Structure Interaction Problem *A. D. Gupta*
4:48p-5:12p	Adjoint Code Differentiation for Hydrodynamic Model Studies *R. J. Henninger, M. L. Rightley & P. J. Maudlin*
5:12p-5:36p	Massively Parallel H-Adaptivity Applications *M. K. W. Wong, J. R. Weatherby & E. A. Boucheron*
5:36p-6:00p	Asymptotic Numerical Method for Shells Using Nonlinear Constitutive Laws *H. Zahrouni, N. Damil & M. Potier-Ferry*

Symposium & organizer(s): G1- Mechanics of Smart Structures. ***H. Irschik (Joh. Kepler U., Austria)***
Session: G1-3 Room: CUB 212 **Time:** M4:00p-6:00p
Chairs: *V. I. Levitas (U. Hannover) & H. Irschik*

4:00p-4:24p	Numerical Simulations of Martensitic Phase Transformations in Plane Strain *G. A. Stiehl*
4:24p-4:48p	Modelling, Analysis and Optimization of Smart Structures by the Finite Element Method. *U. Gabbert*
4:48p-5:12p	Elastoplastic Materials with Martensitic Phase Transition at Finite Strains: Numerical Simulation. *A. V. Idesman, V. I. Levitas & E. Stein*
5:12p-5:36p	Computational Evaluation of Poling Processes *V. G. DeGiorgi*
5:36p-6:00p	Probabilistic Characterization of the Performance of Actively Controlled Smart Structures. *U. O. Akpan & I. R. Orisamolu*

Symposium & organizer(s): H1- Giga Scale Integration Technology: Device, Process and IC Design. ***M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)***
Session: H1-3 Room: CUB B1-5 **Time:** M4:00p-6:00p
Chair: *T. Yamada (NASA)*

4:00p-4:30p	Quantum-DOT Cellular Automata (Invited) *W. Porod*
4:30p-5:00p	Toward Sub-Millimeter Scale All-Optical Switches for Ultrahigh Data-rate Applications (Invited) *D. S. Citrin*
5:00p-5:30p	Atomic Chain Electronics *T. Yamada*
5:30p-6:00p	Web-Based Computing *D. M. Richey, J. D. Finnerty, K. Singhal & J. D. Tauke*

Tuesday Sept. 29

Tuesday Morning: 8:00am-9:00am
PLENARY SESSION A2-1

Symposium & organizer(s): A2- Engineering Science Medal Symposium: Constitutive Models and Penetration Mechanics. In honor of the 1998 Medalist Professor Sol Bodner. ***K. S. Chan & C. Anderson (Southwest Research Institute)***
Session: A2-1 Room: Auditorium **Time:** T8:00a-9:00a
Chair: *C. Anderson (Southwest Research Institute)*

8:00a-9:00a	**Plenary Session:** The Art of Formulating Elastic-Viscoplastic Constitutive Equations *S. R. Bodner*

9:00am-9:30am – Refreshments. Ballroom

Technical Sessions IV
Tuesday Morning: 9:30am-11:30am

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel *Laureate* ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-5 Room: CUB 220 **Time:** T 9:30a-11:30a
Chair: *W. Helfrich (Frei U Berlin)*

9:30a-9:54a	The Life and Death of Bare Viscous Bubbles *G. Debregeas & F. Brochard*
9:54a-10:18a	Macroscopic Properties of Smectic C_G Liquid Crystals *H. Brand, P.E. Cladis & H. Pleiner*
10:18a-10:42a	Interfacial Correlations and Layer Undulations in Self-Assembling Liquid Crystalline Polymers *R. Shashidhar & R.E. Geer*
10:42a 11:06a	Liquid Single Crystal Elastomers (LSCE) *H. Finkelmann, P. Fischer, P., Peter Stein & Pascal Stein*

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-2 Room: Cascade 127 **Time:** T9:30a-11:30a
Chair: *R. Luciano (U. Cassino) & P.M. Suquet (LMA/CNRS)*

9:30a-9:54a	Higher-Order Micromechanics-Based Nonlocal Constitutive Models for Elastic Composites *W. J. Drugan*
9:54a-10:18a	Non Local Constitutive Relations for Heterogeneous Materials *R. Luciano & J. R. Willis*
10:18a-10:42a	Helical Inclusion in an Elastic Matrix *L. I. Slepyan, V. I. Krylov & R. Parnes*
10:42a-11:06a	Microstructure Evolution in Voided Nonlinear Materials *M. Garajeu & P. M. Suquet*

Symposium & organizer(s): B2- Dynamics of Particles in Fluids in Dense Two-Phase Flows. ***C. T. Crowe (WSU)***
Session: B2-1 Room: CUB B7-9 **Time:** T9:30a-11:30a
Chair: *C. T. Crowe (WSU)*

9:30a-10:18a	**Keynote Lecture:** Discrete Particle Simulation of Granular Materials and Multiphase Flows *Y. Tsuji, T. Tanaka & T. Kawaguchi*
10:18a-10:42a	Peristaltic Flow of an Oldroyd-B Fluid in Channels *A. M. Siddiqui, S. Asghar & T. Hayat*
10:42a-11:06a	A Perturbation Study of Particle Dynamics in a Plane Wake Flow *R. W. Davis, T. J. Burns & E. F. Moore*
11:06a-11:30a	Modeling of Complex Two-Phase Flows Using a SPEED Model *X.-Q. Chen*

Symposium & organizer(s): C1- Advanced Modeling in Geomechanics and Minerals Processing. ***H. –B. Muhlhaus (CSIRO, Australia)***
Session: C1-4 Room: CUB B11-15 **Time:** T9:30a-11:30a
Chairs: *Y. Drossinos (JRCEC) & N. D. Cristescu (U. Florida)*

9:30a-9:54a	Complex Dynamics of a Creep-Slip Model of Earthquake Faults *P. Hähner, Y. Drossinos*
9:54a-10:18a	Plastic Waves in Granular Soils *V. Osinov*
10:18a-10:42a	Optimistic/Pessimistic Behaviors of Heterogeneous Body with Statistically Varying Material Properties *M. Hori & H. S. Munashinghe*
10:42a-11:06a	Compaction and Gravitational Creep Flow of Granular Materials *N. D. Cristescu, O. Cazacu & C. Cristescu*
11:06a-11:30a	Discrete Element Modelling of Liquefaction in Calcareous Sand *H. Sakaguchi, & H. B. Mühlhaus*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-4 Room: Auditorium **Time:** T9:30a-11:30a
Chair: *D. Segalman (Sandia)*

9:30a-9:54a	An Efficient, Hybrid Frequency-Time Domain Method for the Dynamics of Large-Scale Dry-Friction Damped Structural Systems *J. Guillen & C. Pierre*
9:54a-10:18a	Modeling, Simulation and Verification of Contact/Impact Dynamics of Flexible Articulated Structures *S. Hariharesan & A. A. Barhorst*
10:18a-10:42a	Minimal Modeling of Multi-Point Contact with Friction in Multiple Rigid-Body Systems *A. L. Nugent & A. A. Barhorst*
10:42a-11:06a	Control of Mechanical System with Nonholonomic Constraints *V. B. Larin*

Symposium & organizer(s): E2- Compressive Failure in Fiber Composites. ***A. Waas (Univ. of Mich.) & C. R. Schultheisz (NIST)***
Session: E2-4 Room: Cascade 125 **Time:** T9:30a-11:30a
Chairs: *S. R. Swanson (U. Utah) & J. Y. Shu (LLNL)*

9:30a-9:54a	Kink Formation and Growth in Fiber-Reinforced Composites *S. Nemat-Nasser & J. McGee*
9:54a-10:18a	Failure Mode Transition in Composites Under Multiaxial Compression *K. Oguni & G. Ravichandran*
10:18a-10:42a	High Strain Rate Compression of Fiber Composites *W. S. Slaughter*
10:42a-11:06a	Scaling of Tensile and Compressive Brittle Failures of Fiber Composites *Z. P. Bažant & E. Becq-Giraudon*
11:06a-11:30a	Crack Interaction Problems in a Fiber-Matrix Composite: Debonding and Broken Fiber. *I. Demir*

Symposium: E4 – Composites, Polymers and Elasticity: Mechanics and Materials Issues in Solid Polymers
S. Ahzi (Clemson) & M. Negahban (Nebraska)
Session: E4-4 Room: CUB 222 **Time:** T9:30a-11:30a
Chairs: *G. Weng (Rutgers) & R. Gregory (Clemson)*

9:30a-9:54a	A Model for Stress Evolution During Thermoset Cure *Y. Mei, A. Wineman & A. F. Yee*
9:54a-10:18a	A Viscoelastic Cohesive Zone Model for Application to Crack Growth in Polymers *D. H. Allen*
10:18a-10:42a	Computer Simulation of Bimodal Elastomer Networks *P. R. von Lockette & E. M. Arruda*
10:42a-11:06a	Microvoid Growth in a Sphere of Elastomeric Material Exhibiting Strain-Dependent Damage *H. E. Huntley & A. S. Wineman*
11:06a-11:30a	Scratching Behavior of Elastomeric PDMS Coatings *S. L. Zhang, A. H. Tsou & J. C. M. Li*

Symposium & organizer(s): F1- - Inelastic Deformation and Failure. Symposium to celebrate Prof. E. Hart's 80th Birthday. ***H. Garmestani (FSU) & F. G. Kollmann (Tech. Hochschule Darmstadt)***
Session: F1-3 Room: CUB 232 **Time:** T9:30a-11:30a
Chair: *A. Khan (U. Maryland)*

9:30a-9:54a	On Non-Proportional Multi-Axial Experiments in Plasticity *A. S. Khan*
9:54a-10:18a	On the Mechanics of the Heart *E. T. Onat*
10:18a-10:42a	Hardening and Strain in Ductile Crystals *J. L. Bassani*
10:42a-11:06a	State Variable Constitutive Modeling Using Physically Based State Variables *D. P. Field*
11:06a-11:30a	Relaxation Behavior and Constitutive Modeling *E. Krempl*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. ***R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)***
Session: F2-4 Room: Cascade 123 **Time:** T9:30a-11:30a
Chairs: *J. P. Hirth (WSU) & R. Thomson (NIST)*

9:30a-9:54a	A Statistical Approach to the Problem of Deformation in Metals *R. M. Thomson & L. E. Levine*
9:54a-10:18a	Dislocation Dynamics in Intermetallics *M. S. Daw*
10:18a-10:42a	Modeling of Dislocations Interacting with a Propagating Crack *H. H. M. Cleveringa, E. van der Giessen & A. Needleman*
10:42a-11:06a	Dislocation Dynamics Simulations in the Presence of Interacting Cracks *I. Demir & A. N. Gulluoglu*
11:06a 11:30a	Laser Induced Deformation Patterns in Films and Surfaces. *D. Walgraef*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-2 Room: CUB 224 **Time:** T9:30a-11:30a
Chairs: *D. G. Sanders (Boeing) & W.C. Simmons (Army Research Office)*

9:30a-9:54a	Aerospace Manufacturing Challenges for Superplastic Forming in the Twenty-first Century *D. G. Sanders*
9:54a-10:18a	Review of Army Interest in Superplasticity *W. C. Simmons*
10:18a-10:42a	Research Toward the Increased Use of Superplastic Forming in Lightweight Structures *M. T. Smith*
10:42a-11:06a	Integrated Design Environment for the Manufacture of SPF Components *N. Chandra, U. Chandra, B. Harvey & J. Shi*
11:06a 11:30a	SPF Application Challenges and Opportunities - A Part Manufacturer Perspective *M. G. Kistner*

Symposium & organizer(s): G1- Mechanics of Smart Structures. ***H. Irschik (Joh. Kepler U., Austria)***
Session: G1-4 Room: CUB 212 **Time:** T9:30a-11:30a
Chairs: *K. Schlacher & H. Irschik (Joh. Kepler U. Austria)*

9:30a-9:54a	Active Vibration Control of Piezoelectricity Based Smart Structures, Theoretical and Experimental Results *K. Schlacher, W. Haas & H. Irschik*
9:54a-10:18a	Optical Fibre Techniques for Structural Measurements *G. Pierce & B. Culshaw*
10:18a-10:42a	Nonlinear Elastic Vibrations of Piezoceramic Shells Subject to Large Driving Voltages *G. A. Altay & M. C. Dokmeci*
10:42a-11:06a	Active Control of Plate Vibrations by Discrete PVDF Actuator and Sensor Segments *L. Gaul & U. Stöbener*
11:06a 11:30a	Ionic Polymer-Metal Composites (IPMC) As Biomimetic Sensors and Actuators-Artificial Muscles *M. Shahinpoor*

Symposium & organizer(s): H1- Giga Scale Integration Technology: Device, Process and IC Design. ***M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)***
Session: H1-4 Room: CUB B1-5 **Time:** T9:30a-11:30a
Chair: *O. Awadelkarim (Penn State)*

9:30a-10:00a	Plasma-Etching-Induced Damage: Impact on Performance and Reliability of Submicron Field-Effect Transistors *O. O. Awadelkarim*
10:00a-10:30a	Current Ramp Testing for In-Process Screening and Monitoring of Electromigration *R. T. Cross, A. Ditali & Z. Hasnain*
10:30a-11:00a	Observation of Degradation Effects on MOSFETs From Interlayer Dielectric Processing. *L. Trabzon & O. O. Awadelkarim*
11:00a-11:30a	An Atomistic Simulator for Thin Film Deposition in Three Dimensions *H. Huang, T. D. de la Rubia & G. H. Gilmer*

Symposium & organizer(s): I1- Biomechanics and Biomathematics. ***K. Campbell (WSU) & C. Martin (Texas Tech)***
Session: I1-1 Room: CUB 214-16 **Time:** T9:30a-11:30a
Chairs: *C. Martin (Texas Tech) & K. Campbell (WSU)*

9:30a-9:54a	Some Modeling Issues in Hill-Based Systems *L. Schovanec*
9:54a-10:18a	A Direct Approach Utilizing Musculoskeletal Dynamics and Neuromuscular Control to Determine Stress Development in Bone *Y. DeWoody & L. Schovanec*
10:18a-10:42a	Comparison Among Putative Myofilament Cooperative Mechanisms Regulating Cardiac Contraction and Relaxation *J. J. Rice, R. L. Winslow & W. C. Hunter*
10:42a-11:06a	Analysis of *in vitro* Sliding Velocities Produced by Mixtures of Different Types of Myosin. *E. F. Pate*
11:06a-11:30a	Differential Equation for Crossbridge Distortion in Muscle Models *K. B. Campbell & M. V. Razumova*

LUNCH - 11:30am - 1:00pm

Technical Sessions V
Tuesday Afternoon: 1:00pm-3:00pm

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel *Laureate* ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-6 Room: CUB 220 **Time:** T 1:00p-3:00p
Chair: *F. Brochard (Inst. Pierre et Marie Cure)*

1:00p-1:24p	Thermomicropolar Flow of a Nematic Liquid Crystal in a Flexible Stenosed Tube *M.N.L. Narasimhan*
1:24p-1:48p	Creating Functional Peptide Architectures at Interfaces *M. Tirrell, G. Fields, E. Yu, S. Ochsenhirt, & T. Pakalns*
1:48p-2:12p	Title to be Provided *N. Berker*

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-3 Room: Cascade 127 **Time:** T1:00p-3:00p
Chairs: *G.W. Milton (U. Utah) & P. P. Castaneda (Pennsylvania)*

1:00p-1:24p	Bounds on the Stress-Strain Relation for Non-Linear Composites. *G. W. Milton*
1:24p-1:48p	Two-Dimensional Composites: Advances in Linear and Nonlinear Conductivity *V. Nesi*
1:48p-2:12p	Bounds for Nonlinear Composites Which Incorporate Morphological Information *D. R. S. Talbot*
2:12p-2:36p	Second-Order Estimates for the Effective Behavior of Nonlinear Polycrystals *M. Bornert & P. P. Castaneda*

Symposium & organizer(s): B2- Dynamics of Particles in Fluids in Dense Two-Phase Flows. ***C. T. Crowe (WSU)***
Session: B2-2 Room: CUB B7-9 **Time:** T1:00p-3:00p
Chair: *C. T. Crowe (WSU)*

1:00p-1:24p	Computational Investigation on Penetration Capability of Sprinkler Sprays with Varying Parameters *S. Nam*
1:24p-1:48p	Numerical Modelling of Bubble Dynamics Using a Fluid Interface Capturing Technique *R. I. Issa*
1:48p-2:12p	Particle-Collision Induced Turbulence in Solid-Liquid Flows *R. Zenit & M. L. Hunt*
2:12p-2:36p	Second-Order Accurate Schemes for Two-Fluid Models of Two-Phase Flow *I. Tiselj & S. Petelin*
2:36p-3:00p	Effect of Suction or Injection on the Periodic Flows of an Oldroyd-B Fluid *T. Hayat, S. Asghar & A. M. Siddiqui*

Symposium & organizer(s): C2 – Computational Methods for Granular Materials. ***B. Loret (Inst. De Mech. De Grenoble) & M. Mehrabadi (Tulane U).***
Session: C2-1 Room: CUB B11-15 **Time:** T1:00p-3:00p
Chairs: *B. Loret & M. Mehrabadi*

1:00p-1:48p	**Keynote Lecture:** Fluid/Particle Interaction in Simulations of Granular Material *P. A. Cundall*
1:48p-2:12p	Numerical Simulation of Large Shear Deformation in Granular Material *S. G. Bardenhagen, J. U. Brackbill & D. L. Sulsky*
2:12p-2:36p	Granular Dynamics Simulation *B. Loret, J. H. Prevost & J. Tantalla*
2:36p-3:00p	Simulation of Two Dimensional Fluid Flow in Soils *E. Masad & B. Muhunthan*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-5 Room: Auditorium **Time:** T1:00p-3:00p
Chair: *R. Zadoks (Texas at El Paso)*

1:00p-1:24p	Stability Analysis of Diamond Turning Manufacturing Processes *D. E. Gilsinn, M. A. Davies, J. Pratt & B. Balachandran*
1:24p-1:48p	Suppression of Regenerative Chatter via Impedance Modulation *D. J. Segalman & E. A. Butcher*
1:48p-2:12p	Optimum Excitation System Mass - Efficiency Design of the D.C. Compound Motor *K. Kowalski, J. Corrales & P. Pedronio*
2:12p-2:36p	

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-4 Room: Cascade 125 **Time**: T1:00p-3:00p
Chairs: *D. P. Warne (U. Tennessee) & P. G. Warne (Maryville College)*

1:00p-1:24p	Boundary Layer Solutions in Elastic Solids *Y-C. Chen, K. R. Rajagopal*
1:24p-1:48p	An Outer and Inner Tensor Product *P. G. Warne*
1:48p-2:12p	Plane Deformations in Incompressible Nonlinear Elasticity *D. P. Warne & P. G. Warne*
2:12p-2:36p	Pure Bending of Incompressible Elastic Plates *D. M. Haughton*
2:36p-3:00p	Instability of an Internally Constrained Hyperelastic Material. *M. F. Beatty & F. Pan*

Symposium: E4 –Mechanics and Materials Issues in Solid Polymers. ***S. Ahzi (Clemson) & M. Negahban (Nebraska)***
Session: E4-5 Room: CUB 222 **Time:** T1:00p-3:00p
Chairs*: M. Boyce (MIT) & S. Ahzi (Clemson)*

1:00p-1:24p	The Role of Long-Term Solutions in Modeling Inelastic Behavior of Solid Polymers. *E. Krempl*
1:24p-1:48p	Inelastic Behavior of Polymers Under High Pressure. *Z. Ma & K. Ravi-Chandar*
1:48p-2:12p	Plastic Behavior of Polyethylene and Related Copolymers in Terms of Uniform and Localized Crystal Slip Processes *R. Séguéla, V. Gaucher-Miri & S. Elkoun*
2:12p-2:36p	Thermomechanical Modeling of Crystallization in Polyethylene for Use in Simulation of Rotational Molding *M. Negahban*
2:36p-3:00p	Application of Drag Reducing Polymer in Energy and Water Saving in Sprinkler Irrigation Systems *M. F. Khalil, A. Elmiligui & F. Naoum*

Symposium & organizer(s): F1- Inelastic Deformation and Failure. Symposium to celebrate Prof. E. Hart's 80th Birthday. ***H. Garmestani (FSU) & F. G. Kollmann (Tech. Hochschule Darmstadt)***
Session: F1-4 Room: CUB 232 **Time:** T1:00p-3:00p
Chairs: *O. Onat (Yale U.) & H. Garmestani (FSU)*

1:00p-1:24p	Thermodynamic Description of Fracture in Inelastic Materials. Similarity with Phase Transitions *V. I. Levitas*
1:24p-1:48p	Influence of Stacking Fault Energy, Grain Size, and Stress State on Deformation Twinning in fcc Polycrystals *S.R. Kalidindi, E. El-Danaf & R.D. Doherty*
1:48p-2:12p	A General Representation of a Titanium Alloy Capturing Reversible and Irreversible Hereditary Behavior *S. M. Arnold, A. F. Saleeb & M. G. Castelli*
2:12p-2:36p	A Micromechanical Model for Metal Creep *W-Y. Shih*
2:36p-3:00p	Phenomenological Modeling of Transient Behavior in Cyclic Loading and Relaxation *H. Garmestani & E. W. Hart*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. ***R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)***
Session: F2-5 Room: Cascade 123 **Time:** T1:00p-3:00p
Chairs: *J. Y. Shu (LLNL) & D. Walgraef (Brussels)*

1:00p-1:24p	Gradient Deformation Models at Nano, Micro and Macro Scales. *E. C. Aifantis*
1:24p-1:48p	Strain Gradient Effects in the Deformation of Metal-Matrix Composites *J. Y. Shu & C. Y. Barlow*
1:48p-2:12p	Computational Modeling of Dislocation Based Gradient Plasticity *L. J. Sluys & Y. Estrin*
2:12p-2:36p	Multiscale Polycrystal Plasticity *R. McGinty & D. L. McDowell*
2:36p-3:00p	

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-3 Room: CUB 224 **Time:** T1:00p-3:00p
Chairs: *J. Will (Boeing Company) & M. K. Khraisheh (King Fahd U.)*

1:00p-1:24p	Advanced Multi-sheet SPF/DB Fabrication *J. D. Will*
1:24p-1:48p	Bulge Forming of Superplastic Sheet Materials Under Strain-Rate Controlled Pressure Profiles *M. K. Khraisheh*
1:48p-2:12p	Retention of Texture in Superplastic Forming of a Hemisphere from Commercial Ti-6A1-V Plate *R. Sundaresan, W. Krishnaswamy, A. K. Singh & K.M. Rao*
2:12p-2:36p	Superplastic Forming of Titanium 6Al-2Sn-2Zr-2Mo-2cr-.2Si *F. S. Gillespie*
2:36p-3:00p	Diffusion Bonding of Superplastic Materials: Theory and Practice *John Pilling, N. Ridley & J. Wang*

Symposium & organizer(s): G2- Phase Transformation in Active Materials. *A. Bhattacharyya (U. Alberta) D. Lagoudas (Texas A & M) & M. Taya (U. Washington)*
Session: G2-1 Room: CUB 212 **Time:** T1:00p-3:00p
Chairs: *M. Wuttig (U. Maryland) & K. Bhattacharya(Calif. Inst. Of Tech)*

1:00p-1:48p	**Keynote Lecture:** Computer Modeling of Mesoscopic Microstructure Formation in Coherent Phase Transformations *A. G. Khachaturyan*
1:48p-2:12p	Martensitic Transformation in Constrained Films *M. Wuttig & A. Roytburd*
2:12p-2:36p	Recoverable Strains in Shape-Memory Polycrystals *K. Bhattacharya & Y-C. Shu*
2:36p-3:00p	New Materials with Unusually Large Magnetostriction *R. D. James*

Symposium & organizer(s): H1- Giga Scale Integration Technology: Device, Process and IC Design. ***M. A. Osman (WSU), K. Mayaram (WSU), O. Awadelkarim (Penn State) & T. Yamada (NASA)***
Session: H1-5 Room: CUB B1-5 **Time:** T1:00p-3:00p
Chair: *P. Pedrow (WSU)*

1:00p-1:30p	Plasma Processing of Electro-Active Polymers and Devices *P. D. Pedrow, R.G. Hoagland, R. Mahalingam & M. A. Osman*
1:30p-2:00p	Short-Channel SOI MOSFETs Threshold Voltage Modeling with Induced Substrate Effects *M. A. Imam & M. A. Osman*
2:00p-2:30p	Third Order Current Cancellation in HBTs *P. K. Wong & B. Pejcinovic*
2:30p-3:00p	Manganese Oxide Films for the Positive Electrode in the Li Secondary Batteries *M. Isai, K. Yamaguchi, T. Nakamura & H. Fujiyasu*

Symposium & organizer(s): I1- Biomechanics and Biomathematics. ***K. Campbell (WSU) & C. Martin (Texas Tech)***
Session: I1-2 Room: CUB 214-16 **Time:** T1:00p-3:00p
Chair: *K. Campbell (WSU)*

1:00p-1:24p	Thermoregulatory Models and Human Responses to the Environment. *R. R. Gonzalez*
1:24p-1:48p	Multisystem Modeling: Pharmacologic and Neural Effects in Cardiovascular Models *R. W. Samsel*
1:48p-2:12p	The Mechanics of Undulatory Swimming: Virtual and Robotic Leeches. *C. E. Jordan, B. M. Stell, R. Tyson & L. J. Fauci*
2:12p-2:36p	The Smoker at Great Depths: Seeking a Unification of Pathophysiology, Mechanics, and Fluid Dynamics. *J. R. Clarke*
2:36p-3:00p	Cardiovascular Model for Gravitational and Accelerative Stress. *K. B. Campbell, R. D. Kirkpatrick & D. E. Swanson*

3:00pm-3:30pm - Refreshments. Ballroom

Technical Sessions VI
Tuesday Afternoon: 3:30pm-5:30pm

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel *Laureate* ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-7 Room: CUB 220 **Time:** T3:30p-5:30p
Chair: *M. Kleman (U. Pierre et Marie Curie)*

3:30p-3:54p	Brownian Motors in the Photoalignment of Liquid Crystals *P. Palffy-Muhoray*
3:54p-4:18p	Microstructural Media in Bundle Space *C. Rymarz*
4:18p-4:42p	Liquid Crystals. From Synthetic Goal to Synthetic Tool *V. Percec*
4:42p-5:06p	Wavelength Doubling Cascade to Möbius Defect Turbulence in a Nematic Liquid Crystal *C. Fradin, H. R. Brand, P.L. Finn & P.E. Cladis*

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-4 Room: Cascade 127 **Time:** T3:30p-5:30p
Chairs: *V. P. Smyshlyaev (University of Bath) & K. Bhattacharya (Caltech)*

3:30p-3:54p	Microscopic Misfit Strains in Polycrystals *O. P. Bruno*
3:54p-4:18p	Homogenization and Bounds for the Overall Elastic Energy of Martensitic Polycrystals *V. P. Smyshlyaev & J. R. Willis*
4:18p-4:42p	A Theory of Thin Films of Martensitic Materials with Application to Microactuators, Part I. *R. D. James*
4:42p-5:06p	A Theory of Thin Films of Martensitic Materials with Applications to Microactuators, Part II. *K. Bhattacharya*
5:06p-5:30p	Continuum Models for Stick-Slip Interface Motion in Shape Memory Tensile Bars *P. Rosakis & J. K. Knowles*

Symposium & organizer(s): B1- Numerical Modeling of Flow around Bluff Bodies. ***S. Parameswaran (Texas Tech), A. Hadid (Boeing), V. Sumantran (GM), R. Sun (Chrysler) & S. S. Ravindran (NASA)***
Session: B1-4 Room: CUB B7-9 **Time:** T3:30p-5:30p
Chair: *R. Sun (Chrysler)*

3:30p-3:54p	Advances Towards Automated Aerodynamic Simulation Using Adaptive Cartesian Grids and Parallel Computers *A.J. Przekwas & Z.J. Wang*
3:54p-4:18p	Computational Analysis for Bluff Body Aerodynamics *T. Han*
4:18p-4:42p	Wind Tunnel Design Optimization Utilizing Analytical Fluids *M. Gleason*
4:42p-5:06p	Using CFD as a Tool in Wind Noise Prediction *G. S. Strumolo*

Symposium & organizer(s): C2 – Computational Methods for Granular Materials. ***B. Loret (Inst. De Mech. De Grenoble) & M. Mehrabadi (Tulane U).***
Session: C2-2 Room: CUB B11-15 **Time:** T3:30p-5:30p
Chairs: *M. Oda (Saitama U.) & A. Anandarajah (Johns- Hopkins U.)*

3:30p-3:54p	Numerical Model for Nonlinear Self-weight Consolidation *A. N. Papanicolaou, B. Muhunthan & P. Diplas*
3:54p-4:18p	Simulation of Micro-Changes in a System of Particles in Silos during Filling *D. Gavrilov & O. G. Vinogradov*
4:18p-4:42p	Numerical Analysis of Higher-Order Continua in Description of Granular Assemblies *K. Bagi & I. Bojtár*
4:42p-5:06p	Study on Elastoplastic Behavior of Granular Model in Terms of Two Dimensional Numerical Tests *Y. Kishino*
5:06p-5:30p	Modeling Split Hopkinson Pressure Bar Tests with a Discrete Element Method *F. V. Donze, S-A. Magnier, L. Daudeville & L. Davenne*

Symposium & organizer(s): D1- Structural Dynamics, Nonlinear Dynamics and Control. ***T. D. Burton & A. Barhorst (Texas Tech)***
Session: D1-6 Room: Auditorium **Time:** T3:30p-5:30p
Chair: *D. Gilsinn (NIST)*

3:30p-3:54p	A New Computational Method in Nonlinear Oscillatory Analysis *M. Singh & L. Dai*
3:54p-4:18p	On Computing the Largest p LCE's of Discrete Dynamical Systems *H. F. von Bremen, F. E. Udwadia & W. Proskurowski*
4:18p-4:42p	Design of Adaptive Fuzzy Sliding Mode Control for Robot Manipulators *A. M. Aledhaibi, K. A. Abdel-Motagely & J-K. Huang*
4:42p-5:06p	A General Theory of Flotation *J. L. Ortiz*
5:06p-5:30p	Acquisition and Tracking with Higher-Order Plant and Nonlinear Regulation of Bode Diagram *B. J. Lurie, A. Ahmed & F. Y. Hadaegh*

Symposium & organizer(s): D2- Control Opportunities in Materials Processing. ***J. Berg (Texas Tech)***
Session: D2-1 Room: CUB B1-5 **Time:** T3:30p-5:30p
Chairs: *T. D. Papathanasiou (U. South Carolina) & X. Ren (Utah State)*

3:30p-3:54p	Modeling Fine-Scale Structures by Integro-Differential Equations *X. Ren*
3:54p-4:18p	Meso-Scale Modeling in Composite Materials using the Boundary Element Method *T. D. Papathanasiou*
4:18p-4:42p	Hydraulic Permeability of Fibrous Media Revisited. *D. S. Clague*
4:42p-5:06p	Microstructural Modeling of the Evolution of Stress and Plastic Strain Fields during Fabrication Cool-Down of Fiber Reinforced IMC's. *S. C. Baxter & M.- J. Pindera*
5:06p-5:30p	Applications of Magnetic Resonance Imaging (MRI) in Process Engineering: Porous Media *M. D. Mantle & L. F. Gladden*

Symposium & organizer(s): E1- Mechanics, Micromechanics and Processing of Composites and Ceramics. ***I. Demir (King Saud U), M. Garnich (PNL) & M. Khraisheh (King Fahd U)***
Session: E1-1 Room: CUB 222 **Time:** T3:30p-5:30p
Chairs: *M. Garnich (PNNL) & M. T. Smith (PNNL)*

3:30p-3:54p	A Multicontinuum Approach to Structural Analysis of Linear Viscoelastic Composite Materials. *M. R. Garnich & A. C. Hansen*
3:54p-4:18p	Functionally Designed Metal-Ceramic Composites Via Solid Freeform Fabrication *M. R. Diaz & A. Bandyopadhyay*
4:18p-4:42p	Net Shaped Al_2O_3/Bioglass Composites for Orthopedic Applications *M. Hanabe, V. Khasbardar & P.B. Aswath*
4:42p-5:06p	Modelling of Mechanics of Composites by Electrical Analogies *A. Szekeres*
5:06p-5:30p	Determination of Glass Transition Temperatures of Adsorbed Stereoregular PMMA by Inverse Gas Chromatography at Infinite Dilution *T. Hamieh, M. Rezzaki & J. Schultz*

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-5 Room: Cascade 125 **Time:** T3:30p-5:30p
Chair: *Y. C. Chen (U. Houston)*

3:30p-3:54p	A Model for Nonlinear Viscoelastic Single Mode Response of an Elastomeric Bushing *A. Wineman, T. VanDyke, S. Shi & S. B. Lee*
3:54p-4:18p	'Springback' and Related Effects in Composites Forming. *A. J. M. Spencer*
4:18p-4:42p	On Finitely Deforming Elastic-Viscoplastic Materials. *J. Casey & D. S. Nath*
4:42p-5:06p	Inflation of an Elastomer Cylinder Which Exhibits Stress Softening Residual Deformation *J. B. Haddow & J. L. Wegner*
5:06p-5:30p	A Model for Nonlinear Viscoelastic Coupled Mode Response of an Elastomeric Bushing *A. Wineman & S. B. Lee*

Symposium: E5 – Viscoelasticity in Composites.
D. Allen (Texas A&M U)
Session: E5-1 Room: CUB 208 **Time:** T3:30p-5:30p
Chairs: *D. Allen (Texas A&M U)*

3:30p-4:18p	**Keynote Lecture:** Viscoelasticity in Composites *R.A. Schapery*
4:18p-4:42p	A Continuum Theory of Cohesive Zone Models *F. Costanzo*
4:42p-5:06p	Micromechanical Analysis of a Granular Viscoelastic Composite *D. Allen*

Symposium & organizer(s): F2- Multi-Scale Modeling of Deformation and Fracture. *R. Thomson (NIST), J. P. Hirth (WSU) & H. M. Zbib (WSU)*
Session: F2-6 Room: Cascade 123 **Time:** T3:30p-5:30p
Chairs: *L. J. Sluys (Delft) & A. Benzerga (Ecole des Mines de Paris)*

3:30p-3:54p	Constitutive Modelling of Inelastic Solids for Plastic Flow Processes Under Cyclic Dynamic Loadings. *W. Dornowski & P. Perzyna*
3:54p-4:18p	Coalescence-Controlled Anisotropic Ductile Fracture *A. Benzerga, J. Besson & A. Pineau*
4:18p-4:42p	Yield Strength Asymmetry Predicted Using Polycrystal Elastoplasticity *N. Barton, P. Dawson & M. Miller*
4:42p-5:06p	Microscopic Expressions of Balance Equations for Macroscopic Continuum Based on Lattice Dynamics *Y. Yasui, K. Shizawa & K. Takahashi*
5:06p-5:30p	A Thermodynamical Theory of Plastic Spin and Internal Stress with Dislocation Density Tensor. *K. Shizawa & H. M. Zbib*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-4 Room: CUB 224 **Time:** T3:30p-5:30p
Chairs: *D. Lesuer (LLNL) & M. Jimenez-Melendo (Universidad de Sevilla)*

3:30p-3:54p	Superplasticity in Nanometals, Nanointermetallics and Nanoceramics: Some Results and Reflections *A.K. Mukherjee, R. S. Mishra & S.X. McFadden*
3:54p-4:18p	Superplastic Behavior of Yttria -Stabilized Zirconia Ceramics *M. Jimenez-Melendo & A. Dominguez-Rodriguez*
4:18p-4:42p	Superplasticity in Laminated Metal Composites *D. Lesuer, C. Syn & O. Sherby*
4:42p-5:06p	Cavitation and Fracture Characteristics of Si3N4p/Al Alloy Composites Exhibiting High-Strain-Rate Superplasticity *H. Iwasaki, M. Mabuchi & K. Higashi*
5:06p-5:30p	Effect of Dopants and Impurities on the High Temperature Mechanical Characteristics of Superplastic Yttria-Stabilized Tetragonal Zirconia *D. M. Owen*

Symposium & organizer(s): F4- Failure Modes in Heterogeneous Materials. ***M. Zikry (NCSU)***
Session: F4-1 Room: CUB 232 **Time:** T3:30p-5:30p
Chairs: *S. R. Kalidindi (Drexel U.) & M. Zikry (NCSU)*

3:30p-3:54p	Role-Specific Experiments for Dynamic Failure of Hybrid Composites *S. Nemat-Nasser & J. Issacs*
3:54p-4:18p	Experimental Determination of Dynamic Crack Initiation and Propagation Fracture Toughness in Thin Aluminum Sheets *D. M. Owen, S. Zhuang, A. J. Rosakis & G. Ravichandran*
4:18p-4:42p	Plastic Deformation and Failure in an A359/SiCp MMC Under High-Strain-Rate Tension *Y. Li, K. T. Ramesh & E. S. C. Chin*
4:42p-5:06p	The Effect of NaCl Concentration on the Low Temperature Hot Corrosion Behaviour of IN-738 and MAR-M-509 *I. M. Allam*
5:06p-5:30-	Effects of Temperature and Pressure in Dynamic Failure *S. Hanim & S. Ahzi*

Symposium & organizer(s): G2- Phase Transformation in Active Materials. ***A. Bhattacharyya (U. of Alberta) D. Lagoudas (Texas A & M) & M. Taya (U. Washington)***
Session: G2-2 Room: CUB 212 **Time:** T3:30p-5:30p
Chairs: *G. P. Carman (U. Calif.) & P. Rosakis (Cornell U.)*

3:30p-3:54p	Hysteresis and Stick-Slip Motion of Phase Boundaries in Dynamic Models of Phase Transitions *A. Vainchtein & P. Rosakis*
3:54p-4:18p	Manufacturing, Testing, and Analysis of Thin Film NiTi Based Systems *K. Ho, P. Jardine & G. P. Carman*
4;18p-4:42p	On Cross-Effects of Phase-Transformation and Plastification in Polycrystalline Materials *E. R. Oberaigner, K. Tanaka, F.D. Fischer & G. Hein*

Symposium & organizer(s): H2- Mechanics and Sensing in Manufacturing Processes. ***A. E. Bayoumi (NCSU)***
Session: H2-1 Room: CUB 214-16 **Time:** T3:30p-5:30p
Chairs: *J. W. Eischen (NCSU) & C. D. Rahn (Clemson U.)*

3:30p-4:18p	**Keynote Lecture:** Automated Tailored Garment Manufacture: The Japanese National Project, *J. E. Berkowitch*
4:18p-4:42p	Engineering Analysis of Limp Material Properties Drives Design of Electromechanical Monitoring System *T. G. Clapp & K. J. Titus*
4:42p-5:06p	Computer Simulation of Fabric Draping *J. W. Eischen & R. Bigliani*
5:06p-5:30p	Iterative Techniques for Fabric Position Control During Folding *S. O. Mast, C. D. Rahn & F. W. Paul*

Conference Banquet
Social Hour - 6:00pm - 7:00pm
Dinner/Program –7:00pm – 10:00pm

Wednesday Sept. 30

Wednesday Morning: 8:00am-9:00am
PLENARY SESSION A3-1

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-1 Room: Auditorium **Time:** W8:00a-9:00a
Chair: *P. P. Castaneda (Pennsylvania)*

8:00a-9:00a	**Plenary Lecture**: Progress and Prospects for the Analysis of Nonlinear Composites *J. R. Willis*

9:00am-9:30am -Refreshments. Ballroom

Technical Sessions VII
Wednesday Morning: 9:30am-11:30am

Symposium & organizer(s): A1- Eringen Medal Symposium. In honor of the Nobel *Laureate* ***Prof. Pierre-Gilles de Gennes. A. C. Eringen***
Session: A1-8 Room: CUB 220 **Time:** W9:30a-11:30a
Chair: *S. Chandrasekhar (Center of Liquid Crystal)*

9:30a-9:54a	Some Recent Mathematical Approaches to the Theory of Liquid Crystals *C. Liu*
9:54a 10:18a	Interactions of Liquid Crystals with Physical Fields in Variational Description *R. Kotowski & E. Radzikowska*
10:18a-10:42a	Remarks About the Dynamics of the Fokker-Planck Equation *D. Kinderlehrer*

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-5 Room: Cascade 127 **Time:** W9:30a-11:30a
Chairs: *R. Weaver (U. Illinois) & R. W. Ogden (U. Glasgow)*

9:30a-9:54a	On Non-Propagation of Acceleration Waves in Anisotropic-Elastic, Plastic Solids *D. Bigoni & B. Loret*
9:54a-10:18a	Surface Wave Propagation in a Pre-Stressed Elastic Body with a Thin Elastic Surface Coating *R. W. Ogden & D. J. Steigmann*
10:18a-10:42a	Wave Propagation in Piezocomposites *F. J. Sabina*
10:42a-11:06a	Radiative Transfer and Diffusion of Elastic Waves in Random Polycrystals *R. Weaver*

Symposium & organizer(s): C2 – Computational Methods for Granular Materials. ***B. Loret (Inst. De Mech. De Grenoble) & M. Mehrabadi (Tulane U).***
Session: C2-3 Room: CUB B11-15 **Time:** W9:30a-11:30a
Chairs: *Y. Kishino (Tohoku U.) & J. Dvorkin (Stanford U.)*

9:30a-9:54a	Efficient Algorithm of Contact Detection for Ellipsoidal and Spheroidal Discrete Elements *S. Sawada*
9:54a-10:18a	Effects of Particle Shapes on DEM-Simulated Behavior of Granular Materials *L. Rothenburg & H. Ouadfel*
10:18a-10:42a	Adaptative Dynamic Relaxation for Granular Mechanics *J-P. Bardet*
10:42a-11:06a	A New Approach to Discrete Element Modeling *M. A. Hopkins*
11:06a-11:30a	Particle Rotation and Couple Stress in Numerical Simulations by Distinct Element Method *K. Iwashita & M. Oda*

Symposium & organizer(s): D2- Control Opportunities in Materials Processing. ***J. Berg (Texas Tech)***
Session: D2-2 Room: Auditorium **Time:** W9:30a-11:30a
Chair: *R. P. Bray (Texas Instruments)*

9:30a-10:18a	**Keynote Lecture:** Optimal Design and Control Problems in the Manufacturing of Advanced Nanoscale Layered Materials *J. A. Burns*
10:18a 10:42a	Modular Feedback Design in Epitaxial Processes *S. C. Warnick & M. A. Dahleh*
10:42a-11:06a	The VMBE System: Virtual Prototyping Within Reach *D. G. Meyer, M. K. Tucker, A. D. Bennett, & A. P. Engelmann*
11:06a-11:30a	Application of Generic Modeling to Plasma Etching Systems *R. P. Bray & R.R. Rhinehart*

Symposium & organizer(s): E1- Mechanics, Micromechanics and Processing of Composites and Ceramics. ***I. Demir (King Saud U), M. Garnich (PNL) & M. Khraisheh (King Fahd U)***
Session: E1-2 Room: CUB 222 **Time:** W9:30a-11:30a
Chairs: *L. V. Smith (WSU) & I. Demir (K. Saud U)*

9:30a-9:54a	Residual Stresses in Embedded Fiber Optic Bragg Gratings *M. B. Christiansen & S. L. Koh*
9:54a-10:18a	Factors Affecting Fiber-Matrix Bond Strength Determination in Composites *R. Kahraman, J. F. Mandell & A. Z. Sahin*
10:18a-10:42a	The Effects of Moisture on the Fatigue Response of Polymer Matrix Composite Materials *L. V. Smith*
10:42a-11:06a	Effects of Fiber Coating on Tensile Properties at High Temperatures of Boron-Aluminum Composites *S.- L. Liu, R. S. Tang, & C..-Y. Shun*
11:06a-11:30a	Mechanical Properties of Tungsten-Silica Composite *D. Jia & K. T. Ramesh*

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-6 Room: Cascade 125 **Time:** W9:30a-11:30a
Chair: *J. Hashemi (Texas Tech)*

9:30a-9:54a	A Class of Exact Solutions in Elastic Dielectrics *K. L. Chowdhury*
9:54a-10:18a	A Galerkin Type Solution for Thermo-Microstretch Elastic Media *S. De Cicco*
10:18a-10:42a	Reflection of Harmonic Waves at the End of a Cylinder with a General Cross Section *H. Taweel & S. B. Dong*
10:42a-11:06a	Determination of Stresses in Shells of Elliptical Cross-Section Under Internal Pressure *Q. S. Zheng, J. Hashemi, J. F. Cardenas-Garcia & C. G.V. Vallabhan*
11:06a-11:30a	A Second-Order Homogenization Method for Finite Elasticity *P. P. Castañeda*

Symposium & Organizer(s): E5 – Viscoelasticity in Composites. ***D. Allen (Texas A&M U)***
Session: E5-2 Room: CUB B1-5 **Time:** W930a-11:30a
Chair: *D. Allen (Texas A&M U)*

9:30a-9:54a	Nonlinear Anisotropic Piezo-Electro-Thermo-Viscoelasticity with Applications to Composites Plates *H.H. Hilton, J.R. Vinson, & S. Yi*
9:54a-10:18a	Constitutive Modeling of Polymeric Composites Undergoing Curing *K. Wang, D.C. Lagoudas, J.D. Whitcomb, & D.H. Allen*
10:18a-10:42a	Numerical Prediction of the Response of a Viscoelastic Laminate to Thermal-Mechanical Loading *S.E. Groves, M.A. Zocher, & S.J. DeTeresa*
10:42a-11:06a	Micromechanics Modeling for Viscoelastic Polymeric Composites - Interphase Effects *L.C. Brinson & F. Fisher*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization, Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-5 Room: CUB 224 **Time:** W9:30a-11:30a
Chairs: *T. Zacharia (ORNL) & R. Sadeghi (MARC)*

9:30a-9:54a	Finite Element Modeling of Superplastic Forming. *R. Sadeghi & Z. Pursell*
9:54a-10:18a	Numerical Simulation Requirements for SPF of an Industrial Titanium Part the First Time Every Time *J. Bennett, K. Haberman & M. Piltch*
10:18a-10:42a	Modeling of Superplastic Forming *T. Zacharia & G. Sarma*
10:42a-11:06a	Control of Superplastic Forming Simulations in a Parallel Processing Environment *K. I. Johnson, M. A. Khaleel, M.T. Smith &P. van. derWalt*
11:06a-11:30a	Parametric Pressure Profiles for Superplastic Sheet Metal Forming *J. A. Lamendola, K. I. Johnson & M. A. Khaleel*

Symposium & organizer(s): F4- Failure Modes in Heterogeneous Materials. ***M. Zikry (NCSU)***
Session: F4-2 Room: CUB 232 **Time:** W9:30a-11:30a
Chairs: *S. E. Schoenfeld (US ARL) & M. Ortiz (Caltech)*

9:30a-9:54a	Three-Dimensional Simulation of Dynamic Decohesion in Layered Structures *M. Ortiz*
9:54a-10:18a	Microstructural Failure Modes in Heterogeneous Materials *M. A. Zikry & K. Jagannadham*
10:18a-10:42a	Dimple Fracture Analysis Under Different Constraint Conditions *M. Kikuchi, M. Geni & A. Muramatsu*
10:42a-11:06a	An Adaptive Global-Local Analysis of Heterogeneous Materials with Evolving Microstructural Damage *S. Ghosh, K. Lee & S. Moorthy*
11:06a-11:30a	

Symposium & organizer(s): G2- Phase Transformation in Active Materials. ***A. Bhattacharyya (U. of Alberta) D. Lagoudas (Texas A & M) & M. Taya(U. Washington)***
Session: G2-3 Room: CUB 212 **Time:** W9:30a-11:30a
Chairs: *M. Taya (UW) & A. Bhattacharyya (U. Alberta)*

9:30a-9:54a	Thermomechanical Finite Element Analysis for Axisymmetric Shape Memory Alloy Structures, *J. G. Boyd & M. Capanu*
9:54a-10:18a	Simulated Superelastic Response of NiTi SMA Wires for Orthodontic Applications *D. Raboud, M. G. Faulkner & A. W. Lipsett*
10:18a-10:42a	Finite Element Modeling of Phase Transformation in Shape Memory Alloy Wires with Variable Material Properties *A. Bhattacharyya, J. Amalraj & G. Faulkner*
10:42a-11:06a	Martensitic Transformation in Elastic-Plastic Materials Subjected to a Complex Loading Path, *Y.H. Wen, G. Reisner, F.D. Fischer & K. Tanaka*
11:06a-11:30a	Micromechanic Modeling of Shape Memory Alloys and Their Composites *M. Taya, A.H.Y. Lue, Y. Tomota & K. Inoue*

Symposium & organizer(s): H2- Mechanics and Sensing in Manufacturing Processes. ***A. E. Bayoumi (NCSU)***
Session: H2-2 Room: CUB 214-16 **Time:** W9:30a-11:30a
Chairs: *Y. S. Lee (NCSU) & O. A. Abu Zeid (U. United Arab Emirates)*

9:30a-9:54a	Geometric Modeling and Tool Placement Problems for Multi-Axis CNC Complex Surface Machining. *Y.-S. Lee*
9:54a-10:18a	On the Mechanistic Modeling of Milling Cutting Forces: Hole Making Using an End-Mill Cutter *M. K. Khraisheh & A. E. Bayoumi*
10:18a-10:42a	Experimental Modeling of The Machining Characteristics of EDMed AISI T1 High Speed Steel *O.A. Abu Zeid & M. Y. Bassiouni*
10:42a-11:06a	A New Model for Chip Dynamics in Machining *T. J. Burns, M. A. Davies & C. J. Evans*
11:06a-11:30a	Mathematical Background of CAM System for Sculptured Part Surface Machining on Multi-axis NC Machine Tool. *S. P. Radzevich*

LUNCH - 11:30am - 1:00pm

Technical Sessions VIII
Wednesday Afternoon: 1:00pm-3:00pm

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist **Prof. John R. Willis.** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-6 Room: Cascade 127 **Time:** W1:00p-3:00p
Chairs: *S. Nemat-Nasser (UC-San Diago) & J.L. Bassani (U. Penn)*

1:00p-1:24p	Lattice Incompatibility and Nonlocal Crystal Plasticity *J. L. Bassani*
1:24p-1:48p	A Theory of Single Crystal Plasticity with Microstructure *M. Ortiz & E. Repetto*
1:48p-2:12p	Finite Plastic Flow of Granular Materials *S. Nemat-Nasser*
2:12p-2:36p	A Generalized Peierls-Nabarro Model of a Dislocation in a Discrete Lattice *A. B. Movchan, J. R. Willis & R. Bullough*

Symposium & organizer(s): C2 – Computational Methods for Granular Materials. ***B. Loret (Inst. De Mech. De Grenoble) & M. Mehrabadi (Tulane U).***
Session: C2-4 Room: CUB B11-15 **Time:** W1:00p-3:00p
Chairs: *L. Rothenburg (U. Waterloo) & B. Loret (Inst. De Mech. De Grenoble)*

1:00p-1:24p	Deformation Mechanisms in Granular Materials. *M. R. Kuhn*
1:24p-1:48p	A Network Model for Powder Densification During Initial Stage Sintering *F. Parhami & R. M. McMeeking*
1:48p-2:12p	Mechanics and Physics of Clean and Contaminated Clays. *A. Anandarajah*
2:12p-2:36p	Two Practical Problems of Particulate Mechanics *J. P. Dvorkin & R. Bachrach*
2:36p-3:00p	Time-Dependent Subloading Surface Model *K. Hashiguchi*

Symposium & organizer(s): D2- Control Opportunities in Materials Processing. ***J. Berg (Texas Tech)***
Session: D2-3 Room: Auditorium **Time:** W1:00p-3:00p
Chair: *C. Doumanidis (Tufts U.)*

1:00p-1:24p	Verification of Bond Quality Improvement for Closed Loop Temperature Control of the In-Situ Thermoplastic Composite Tape-Laying Process. *W-C Sun, S. C. Mantell, & K. A. Stelson*
1:24p-1:48p	Extrusion Process Control: Modeling, Identification, and Control *B. Tibbetts & J. T. Wen*
1:48p-2:12p	Parameter Sensitivity and Robust Feedback Controllers for Consolidation Processing of Titanium Matrix Composites *R. Vancheeswaran , H. N. G. Wadley, D.G. Meyer, T. Piatt & R.L. Kosut*
2:12p-2:36p	Thermal Control of Materials Processing in Solid Freeform Fabrication Techniques *N. Fourligkas & C. Doumanidis*
2:36p-3:00p	Material Deposition Control in Thermal Solid Freeform Fabrication Methods *Y-M. Kwak & C. Doumanidis*

Symposium & organizer(s): E1- Mechanics, Micromechanics and Processing of Composites and Ceramics. ***I. Demir (King Saud U), M. Garnich (PNL) & M. Khraisheh (King Fahd U)***
Session: E1-3 Room: CUB 222 **Time:** W1:00p-3:00p
Chairs: *M. Khraisheh (K. Fahd U) & A. C. Hansen (Wyoming)*

1:00p-1:24p	Analytical Determination of Plastic Deformation During Continued Cyclic Loading of Composite Spheres and Cylinders *A. Bhattacharyya & E.J. Appiah*
1:24p-1:48p	Natural Vibration Characteristics of Rotating Adhesively Bonded Cantilever Plates *A.K. Yavuz & T. Kotil*
1:48p-2:12p	A Rigorous Theory for the Elastostatic Analysis of Laminated Beams. *Z.S. Abduljabbar*
2:12p-2:36p	Synthetic Constitutive Data for Random Composites *J.B. Aidun, D. C.S. Lo & M.D. Rintoul*
2:36p-3:00p	Structural Response of Laminated Composite Shells Subjected to Blast Loadings *H. S. Türkmen & Z. Mecitoğlu*

Symposium & organizer(s): E3 – Topics in Theoretical and Applied Elasticity. ***Y. C. Chen (U. Houston) & D. Steigmann (UC-Berkeley)***
Session: E3-7 Room: Cascade 125 **Time:** W1:00p-3:00p
Chairs: *A. Wineman (U. Mich.) & J.F. Cárdenas-Garcia (Texas Tech)*

1:00p-1:24p	Mechanical Response of Dry and Wet Sand to High Strain Rate Loading *W. H. Wilson, D. G. Tasker, R. D. Dick, P. K. Gustavson, J. S. Dieter & R. J. Lee*
1:24p-1:48p	The Practical Use of the Hole Method Using Moire. *J. F. Cárdenas-Garcia & J. E. Verhaegh*
1:48p-2:12p	Singular Problems in Elasticity: Linear vs. Nonlinear Theory. *A. R. Aguiar&R.L. Fosdick*
2:12p-2:36p	Experiments and Modeling of Nonlinear Coupling Effects in Elastomeric Bushings *J. Kadlowec, A. Wineman & G. Hulbert*
2:36p-3:00p	Evaluation of Viscoelastic Characteristics of Soft Stringy Foods. *Y. Nakajo*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization , Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-6 Room: CUB 224 **Time:** W1:00p-3:30p
Chair: *M. Khaleel (PNL)*

1:00p-1:24p	Transformation Superplasticity of a Whisker-Reinforced Titanium Matrix Composite *C. A. Schuh and D. C. Dunand*
1:24p-1:48p	A Parametric Study of Void Growth in Superplastic Deformation *T. A. Khraishi , H. M. Zbib & M. Khaleel*
1:48p-2:12p	Constitutive Modeling of Deformation and Damage in Superplastic Materials *M. A. Khaleel & H.M. Zbib*
2:12p-2:36p	A Phenomenological Model for Aluminum Based Superplastic Materials *F. Booeshaghi, H. Garmestani & R. Vaghar*
2:36p-3:00p	An Investigation on the Densification and the Sinter Forging Characteristics of Alumina-Magnesia Composites *S. Shah, A.H. Chokshi & R. Raj*
3:00p-3:24p	The Characteristics of Deformation and Cavitation in Coarse-Grained Al-4.5Mg Alloys Exhibiting Superplastic-Like Behavior *H. Iwasaki, H. Hosokawa, T. Mori, T. Tagata, M. Mabuchi & K. Higashi*

Symposium & organizer(s): F4- Failure Modes in Heterogeneous Materials. ***M. Zikry (NCSU)***
Session: F4-3 Room: CUB 232 **Time:** W1:00p-3:00p
Chairs: *K. T. Ramesh (Johns Hopkins) & G. Ravichandran (Caltech)*

1:00p-1:24p	Modeling Dynamic Spall Failure in Metals *G. Ravichandran & W. Tong*
1:24p-1:48p	An Investigation on Failure Waves From a Viewpoint of Phase Change. *Z. Chen*
1:48p-2:12p	Computation of Flexural Crack Width in Fibre Reinforced Concrete Members *I. I. Pandya, R. H. Shah & S. K. Damle*
2:12p-2:36p	The Nonlinear Behavior of Trusses Under Earthquake. *B. A. Ovunc*

Symposium & organizer(s): G2- Phase Transformation in Active Materials. **A. Bhattacharyya (U. of Alberta) D. Lagoudas (Texas A & M) & M. Taya (U. Washington)**
Session: G2-4 Room: CUB 212 **Time:** W1:00p-3:00p
Chairs: *G. J. Weng (Rutgers U.) & A. Bhattacharyya (U Alberta)*

1:00p-1:24p	Micromechanical Modeling of the Transformation Induced Plasticity in Steels *M. Cherkaoui & M. Berveiller*
1:24p-1:48p	Deformation Field Evolution During Transformation of Single Crystal SMA *Q-P. Sun*
1:48p-2:12p	Interaction of Plasticity with Phase Transformation in SMA Actuators *D. C. Lagoudas & Z. Bo*
2:12p-2:36p	Influence of the Applied Stress on the Thermally-Induced Phase Transformation in Shape-Memory Alloys. *Z. K. Lu & G.J. Weng*

Symposium & organizer(s): H2- Mechanics and Sensing in Manufacturing Processes. ***A. E. Bayoumi (NCSU)***
Session: H2-3 Room: CUB 214-16 **Time:** W1:00p-3:00p
Chairs: *A. E. Bayoumi (NCSU) & K. Awan (U. of Tech.)*

1:00p-1:24p	Feature Based CAD System For Axi-Symmetrical Objects *K. A. Awan & S. Suliman*
1:24p-1:48p	A New CAE Interface in Virtual Shared Space *Y. Wada, S. Yoshimura, G. Yagawa, K. Susa & T. Kowalczyk*
1:48p-2:12p	Breaking Mechanism of Chips in Intermittently Decelerated Feed Drilling *K. Sakurai & K. Adachi*
2:12p-2:36p	Gear Finishing Technology and Design of Gear Shaving Cutter *S. P. Radzevich, V. A. Palaguta & E. D. Goodman*

3:00pm-3:30pm -Refreshments. Ballroom

Technical Sessions IX
Wednesday Afternoon: 3:30pm-5:30pm

Symposium & organizer(s): A3- Prager Medal Symposium. In honor of the 1998 Prager Medalist ***Prof. John R. Willis.*** ***P. P. Castaneda (U. of Pennsylvania)***
Session: A3-7 Room: Cascade 127 **Time:** W3:30p-5:30p
Chairs: *A.J. Rosakis (CalTech) & N. V. Movchan (U. Bath)*

3:30p-3:54p	Nonlinear Fracture Mechanics of Piezoelectric Ceramics. *C. C. Fulton & H. Gao*
3:54p-4:18p	Mathematical Modelling of Fracture in Fibre-Reinforced Ceramic Materials *N. V. Movchan & J. R. Willis*
4:18p-4:42p	Dynamic Shear-Dominated, Intersonic Crack Growth in Bimaterial and Layered Systems *A. J. Rosakis*
4:42p-5:06p	On the Analysis of Dynamic Unsteady Crack Growth in Elastic Material *J. R. Walton & T. Leise*

Symposium & organizer(s): D2- Control Opportunities in Materials Processing. ***J. Berg (Texas Tech)***
Session: D2-4 Room: Auditorium **Time:** W3:30p-5:30p
Chair*: J. M. Berg (Texas Tech)*

3:30p-3:54p	Advanced Automation Technology Needs and Applications in the Steel Industry *M. S. Dudzic*
3:54p-4:18p	Bar Lapping Process Modeling and Control *Y. Mei & K. A. Stelson*
4:18p-4:42p	A Level Set Framework for Calibration of Low-Order Etching and Deposition Models *J. M. Berg*
4:42p-5:06p	Feedback Control of Shape Memory Alloy Actuators. *C. Dickinson & John T. Wen*
5:06p-5:30p	Forging of a γ-TiAl Automobile Exhaust Valve Using Optimal Conditions *W. M. Mullins, S. Medeiros, L. D. Smith, J. M. Berg, W. G. Fraizer, & J. C. Malas*

Symposium & organizer(s): F3 – Superplasticity and Superplastic Forming: Characterization , Modeling and Applications. ***M. Khaleel (PNL), M. T. Smith (PNL) & C.H. Hamilton (WSU)***
Session: F3-7 Room: CUB 224 **Time:** W3:30p-5:30p
Chair: *M. Khaleel (PNL)*
Panel Discussion: Research Needs

Symposium & organizer(s): F4- Failure Modes in Heterogeneous Materials. ***M. Zikry (NCSU)***
Session: F4-4 Room: CUB 232 **Time:** W3:30p-5:30p
Chairs: *A. Abdul-Latif (Paris 8 Université) M. Zikry (NCSU)*

3:30p-3:54p	The Giga cycle Fatigue of Nickel-Base Alloys. *C. Bathias & J. Bonis*
3:54p-4:18p	Influence of Cold-Working and Aging Heat Treatment on Strength and Ductility *S.R. Kalidindi, E.M. Shaji & R. D. Doherty*
4:18p-4:42p	Anisotropic Viscoplasticity in Rolled Aluminum Plate: Experiments and Simulations, *M. P. Miller, H. P. Gunawardane & N. R. Barton*
4:42p-5:06p	Inhomogeneous Texture Evolution During Explosive Forming. *S. E. Schoenfeld*
5:06p-5:30p	Study of the Local and Global Responses of Heterogeneous Polycrystals Under Non-Proportional Cyclic Loading *J. P. Dingli, A. Abdul-Latif & K. Saanouni*

Symposium & organizer(s): G2- Phase Transformation in Active Materials. ***A. Bhattacharyya (U. of Alberta) D. Lagoudas (Texas A & M) & M. Taya (U. Washington)***
Session: G2-5 Room: CUB 212 **Time:** W3:30p-5:30p
Chair: *V. I. Levitas (U. Hannover)*

3:30p-3:54p	Global Criterion of Phase Transition in Inelastic Materials Based on Stability Analysis *V. I. Levitas*
3:54p-4:18p	Micromechanics Modelling and Parametric Study in Microstructure Design of SMA Composite *Q-P. Sun.*
4:18p-4:42p	Theory of Pseudoelasticity Accounting for the Asymmetry in Tension-Compression of Shape Memory Alloys *C. Lexcellent, J. Rejzner, S. Miyazaki & P. Robinet*
4:42p-5:06p	Thermomechanical Response of Polycrystalline SMAs Under Cyclic Loading: Modeling and Experiments of Minor Hysteresis Loops *Z. Bo & D. C. Lagoudas*
5:06p-5:30p	Temperature Induced Phase Transformation of an SMA Strip *A. K. Davis & N. R. Sottos*

Symposium & organizer(s): H2- Mechanics and Sensing in Manufacturing Processes. ***A. E. Bayoumi (NCSU)***
Session: H2-4 Room: CUB 214-16 **Time:** W3:30p-6:00p
Chairs: *M. K. Khraisheh (King Fahd U) & M. Ketabchi (Tohoku U.)*

3:30p-3:54p	Recent Trends in Manufacturing Education *A. E. Bayoumi*
3:54p-4:18p	Three Dimensional Analysis of Metal Flow in Extrusion of Non-Symmetrical Section Based on Upper Bound Theorem *M. Ketabchi, K. Ikeda & T. Murakami*
4:18p-4:42p	Effects of Prebulging and Maximum Chamber Pressure in Hydromechanical Deep-Drawing: a Finite Element Analysis *S. H. Zhang, M. J. Jensen, D. C. Kang & J. Danckert*
4:42p-5:06p	Relationship Between Joint Performance and Heat Input in Friction Welding *T. Sawai , K. Ogawa, T. Kurozawa & Y. Suga*
5:06p-5:30p	Growth and Distortion of Parts Due to Application of Fasteners *S. Mahanian*
5:30p-5:54p	On Prediction of Fracture in Metal Forming Operations *S. Alexandrov*

CONFERENCE INFORMATION

Session Venues
The welcome, keynote and plenary lectures, welcome reception, farewell banquet, and the poster sessions will take place in the Compton Union Building (*CUB*) on the Washington State University campus in Pullman, Washington. Also the registration and service desks and the message center are found in the CUB.

Contact Address before the Conference
If you have questions about the conference before the conference week, or for questions regarding registration, payments, accommodation, the accompanying persons program, or the tours before and after the conference please contact:

SES Conference
Conferences and Institutes
Washington State University
PO Box 945222
Pullman, WA 99164-5222 USA

Phone: 509-335-3530
800-942-4978 in the US
Fax: 509-335-0945
Email: wsuconf@wsu.edu

Information on the conference is also available on the World Wide Web (www):
http://www.mme.wsu.edu/ses98.htm
http://www.eus.wsu.edu/c&i/programs/SES98.htm

Conference Pack
Each participant will receive a Conference Pack containing the name badge, the final conference program, a list of participants, admission tickets for the welcome reception and farewell banquet. Your personal badge is your admission ticket to all the sessions. Kindly wear your badge at all times. Your Conference Pack is available at the registration desk on the second floor mezzanine of the Compton Union Building.

Every participant will receive a copy of the "**Book of Abstracts**" upon registration at the conference site. It contains copies of the keynote presentations and abstracts of the presented papers. Additional copies may be purchased at the reception desk

Aids to Disabled Persons
All buildings used for conferences on the Washington State University campus have facilities for disabled people. Accommodations for individuals who qualify under the Americans with Disabilities Act are available upon request. Please contact Conferences and Institutes at least 15 days in advance of the event.

Banking
The Bank of Pullman has a branch office in the Compton Union Building. Travelers' checks may be cashed there and cash advances may be drawn against your MasterCard, Visa or Discover bankcards. There is no foreign currency exchange in Pullman. We urge you to exchange your money at the international airport where you enter the United States.

Computers
The 1998 SES conference will have a room in the Compton Union Building with computers connected to the Internet so delegates may have access to email.

Telecommunications /Copies & Faxing
There are public telephones in the Compton Union Building. Copy and fax services are available for a fee on the ground floor of the Compton Union Building (CUB).

Messages
Messages may be left with Conferences & Institutes at 509-335-3530 or faxed to 509-335-0945. Messages, faxes, and email to conference participants sent in care of C&I will be delivered to the *CUB* registration desk and posted at the message board. Attendees are urged to check the message board frequently.

Post Office
A United States Post Office is located on the ground floor of the Compton Union Building (CUB). It is open from 9am to 4:30pm Monday through Friday. Packaging materials are sold at the post office.

Travel Agency
The Travel Studio is a full-service travel agency located on the ground floor of the CUB. Their hours are from 0730 to 1600. Telephone: 509 332-1212. FAX: 509 334-0563. E-mail: travelstudio@TurboNET.com.

Scholarships
The conference organizers attach great importance to a strong scientific representation from the different regions of the U.S. As the shortage of funds impedes the participation of many students, the conference organizers have arranged to help students with an evident need for assistance regarding costs of registration, board and lodging. **(Contact the SES Conference for more details)**

Local Information

Pullman, Washington sits among gently rolling hills of the great Columbia Plateau east of the Cascade Mountains. This is a rich agricultural area known as the Palouse. The Palouse, a French word meaning "green lawn," produces mainly soft white winter wheat, dry peas and lentils. Rich soil, combined with a climate that is transitional between typical grassland and woodland, makes for successful dry land farming with yields routinely topping 100 bushels per acre. Washington State University typically enrolls about 17,000 students. The university offers 150 degrees through eight colleges including agriculture, business, education, engineering, liberal arts, pharmacy, sciences, and veterinary medicine.

Climate
In September, evenings and nights are in the 10-15 Celsius range and temperatures can be 18-25 Celsius during the day. Pullman's elevation is 2,300 feet (700 m) above sea level and the humidity is very low. Occasional showers can be expected.

Clothing
Dress in the Pacific Northwest is generally casual. The organizers suggest that you bring a warm sweater or jacket for chilly evenings and an umbrella or a raincoat. Walking shoes are recommended for tours and excursions.

Dining
Meals are not included in the conference registration fee with the exception of the welcome reception and farewell banquet. Some motels include a generous continental breakfast in the room rate; that is noted as appropriate on the accommodation information. There are some lunch and snack places in the Compton Union Building. Further information about dining in the Pullman area will be provided at the conference information desk.

Local Transportation
Pullman Transit offers regular fixed routes in Pullman only. Buses operate from 0650 to 1850. Service between Pullman, WA, and Moscow, ID, is provided by Wheatland Express, which offers fixed routes. Local shuttle service for conference participants will operate at fixed times between hotels listed in this brochure beginning Sunday, July 6. Schedules will be posted at all motel registration desks. Many of the motels provide free shuttle from the hotel to campus and pick up free at the Pullman/Moscow Airport. Many of the hotels and the University residence halls are within walking distance of the meeting locations.

Medical Care
Medical care in Pullman is of a high standard and the Pullman Hospital is located on the Washington State University Campus. Addresses and telephone numbers of hospitals and health care providers are available at the Conference Information Desk and the Accompanying Persons Hospitality Room.

Passports, Visas
Please contact the nearest US embassy or consulate to find out the passport and visa requirements for entry into the United States. It would be advisable to explain the purpose of your visit to the US consulate to obtain the appropriate visa.

Time Pullman, WA is on Pacific Time (GMT -7 hours).

SOCIAL EVENTS

Welcoming Reception – A Taste of Washington
The Opening reception will celebrate the beauty and bounty of Washington State. Foods, soft drinks, micro-beers and wines of the region will tempt your taste buds. This event is included in the participant and the accompanying persons registration fee.
(Sunday, Sept. 27, 5pm-9pm, Lewis Alumni Center)

Banquet: Tuesday 6pm-10pm. A taste of the Northwest cuisine, with choices of Salmon and Steak, wine and cheese.

Accompanying Persons Program
A variety of tour programs have been arranged specially for accompanying person. Please note that you will need a ticket for each tour. Indicate participation on the registration form. *All prices are TBD.* ***The registration deadline for these tours is July 25, 1998***. If there are less than 20 persons on any tour, Conferences & Institutes reserves the right to cancel the tour, in which case your money will be refunded. Please indicate the number of tickets needed for your selected tours on the registration form and include payment. A refund will be made for any tours canceled due to low enrollment.

Guests of conference participants may attend special conference events by registering as an accompanying person. The accompanying person registration fee of $65 includes attendance at the Sunday evening opening reception, the Banquet and Coffee Breaks.

Tours
A Paradise Called the Palouse (10/1/98)
Take to the back roads and cross the Snake River at Lower Granite Dam. Here observe the locks for ships and barges traveling this waterway to and from the Columbia River. You may see some fish migrating up the river at the visitor center. Enjoy a picnic box lunch at Lyons Ferry Park located on the Snake River. Next, stop at spectacular Palouse Falls. The waterfall here seems to appear out of the prairie as it tumbles 196 feet over the steep basalt cliffs deposited millions of years ago. Travel to the top of Steptoe Butte, looming above the panoramic Palouse near the heart of the region. From here, the agricultural crops of this fertile area look like a giant patchwork quilt with many colors and textures. Cost: $49.00 /person
Minimum participants: 27.....Maximum: 45

Nez Perce National Historic Park and Dworshak National Fish Hatchery (9/25/98)
Visit the Nez Perce National Historic Park and Visitor Center where tribal culture is explained with a series of displays and slide shows. The Nez Perce was one of the most powerful tribes in the Inland Northwest. This tour explores the history and culture of the tribe. Personnel from the visitor's center and tribal elders will join our group for special presentations and lunch. Then, travel on to the Dworshak National Fish Hatchery operated by the Department of Interior's Fish and Wildlife Service. Here, view various stages of growth of the fish as they are readied for entry into the Columbia and Snake River.
Cost: $45.00 /person
Minimum participants: 27.....Maximum: 45

Jet Boating in Hell's Canyon (9/26/98)
Travel south to America's deepest gorge, Hell's Canyon, where your group will ride jet boats down the Snake River. This is an unforgettable trip through the beautiful and rugged country of the Northwest. You will roar 57 miles up the Snake River to explore the site and learn about the legends of an early 1900's mining town. Lunch is an all-you-can-eat Western barbecue at Heller Bar overlooking the Snake River
Cost: $95.00 /person
Minimum participants: 27.....Maximum: 90

PAPERS AND POSTERS

Punctuality
In a conference such as this with many speakers, it is essential that the moderator and the speakers adhere closely to the timetable of each session. Please be punctual. Do not use more than your allocated time. Out of fairness to all speakers and to the other session participants, session moderators are charged with the responsibility to see that the schedule is observed

Oral Presentations
Each speaker will have 24 minutes for his/her oral presentation. Each Keynote lecturer will have 48 minutes. Speakers are urged to contact the moderator of their session as soon as possible after arrival.

Slides or overhead transparencies are recommended for use in oral presentations. Please make your visual aids carefully. People should see and understand your presentation even in the back of the room. There should be no transparencies of typed information.

Audio-visual aids
Overhead projectors for transparencies, 35mm slide projectors, and projection screens will be available in all meeting rooms free of charge. Flip charts or the equivalent will be free of charge. Additional equipment will be available on request for a charge. Visa, MasterCard or cash will be accepted to pay for additional equipment you request. Videocassette players (VHS only) will be available on request. If you need to use video or other special equipment, please contact the Conference Office a month in advance and give full details.

Guidelines for Poster Presentations
All posters will be displayed in the Compton Union Building. Each poster will be assigned to a numbered panel. Authors should personally be present during their assigned time. The preferred language of your poster is English.

The posters will be grouped according to the appropriate Topic. Authors will mount their posters. The set-up times are one hour prior to the scheduled presentation time. Posters must be dismantled within one hour following the scheduled presentation time to allow the next group of authors enough time to set up. A room is reserved in the Compton Union Building for the temporary storage of poster materials.

The panel display will be 121 cm wide x 102 cm high. Pins will be available to put up the posters in the poster session exhibit room. You should design your poster accordingly. Illustrations must be drawn clearly. The text should be readable at a distance of 1.5 meters. There will be a table in front of the panel to display any material the authors wish to distribute to the delegates.

ACCOMMODATIONS IN THE PULLMAN AREA

You are responsible for making your own reservations for lodging. Prices listed for motels have been arranged for this conference. Mention the SES '98 conference when you reserve. Add 7.5% sales tax in Washington and 5% sales tax in Idaho to quoted prices. (For help, you may fill-out the enclosed "**Assistant Request Form**")

Pullman, Washington

Holiday Inn Express **(Highly recommended!)**
509-334-4437 Fax: 509-334-4447
1190 SE Bishop Blvd., Pullman, WA 99163
Conf. Rates: $59.00 1-4 people, 1-2 beds
—inside swimming pool
—includes continental breakfast
—free shuttle service to/from airport & WSU campus

Quality Inn Paradise Creek **(Highly recommended!)**
509-332-0500 Fax: 509-334-4271
1050 SE Johnson Avenue, Pullman, WA 99163
Conf. Rates: $48.50 single
$55 2-4 people, 2 beds
—outside swimming pool
—includes continental breakfast
—free shuttle service to/from airport & WSU campus

American Travel Inn Motel
509-334-3500 , Fax: 509-334-0549
515 S Grand Ave.,
Pullman, WA 99163
Conf. Rates: $38 single, $42 double
(*We recommend that you have a car to commute locally*)

Compton Union Building (CUB)
509-335-9444 Fax: 509-335-4803
Washington State University,
Pullman, WA 99164-7204
Conf. Rates: $40 single
$45 2 people, 2 beds
$50 3 people, 2 beds
$55 4 people, 2 beds
-- Parking permits included in fee

Best Western Heritage Inn
509-334-2555 Fax: 509-334-2555
Davis Way, Pullman, WA 99163
Conf. Rates: $46 King-sized bed
$46 Two Queen-sized beds
—inside swimming pool
—includes continental breakfast
(*We recommend that you have a car to commute locally*)

Manor Lodge Motel
509-334-2511 (no fax)
455 SE Paradise,
Pullman, WA 99163
Conf. Rates: $37 single
$42 double
$47 2 people, 2 beds
$50 3 people, 2 beds
$55 3 people, 2 beds
(*We recommend that you have a car to commute locally*)

Nendels Inn
509-332-2646 Fax: 509-332-2525
915 SE Main, Pullman, WA 99163
Conf. Rates: $39 single
$49 double
$54 3 people, 2 beds
$59 4 people, 2 beds
(*Within walking distance for physically active persons.*)

Moscow, Idaho (Moscow, Idaho is eight miles east of Pullman.)

University Inn, Best Western **(Highly recommended!)**
800-334-7234
or 208-882-0550 Fax: 208-883-3056
1516 Pullman Road, Moscow, ID 83843
(across from the University of Idaho)
Conf. rates: $59.50 single
$69.50 2-4 people, 2 beds
—inside swimming pool
—includes continental breakfast M-F
—free shuttle service to/from airport

Super 8 Motel
208-883-1503 Fax: 208-883-4769
175 Peterson, Moscow, ID 83843
Conf. Rates: $39 single
(includes sales $43 double
tax) $47 2 people, 2 beds
$52 3 people, 2 beds
$56 4 people, 2 beds
$59 3 people, 3 beds
(*We recommend that you have a car to commute to conference*)

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Abstracts

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Symposium A1

Eringen Medal Symposium In honor of the Nobel Laureate
Prof. Pierre-Gilles de Gennes
Organizer
A. C. Eringen, USA

Session: A1-1 Room: Auditorium, **Time:** M8:30a-9:30a
Chair: ***T. Chang (MIT)***

Tentative Reflections on Powder Mechanics

de Gennes, P-G.
Ecole Supérieure de Physique et de Chimie Industrielles, France

The statics of dry granular materials has recently been a matter of dispute. Traditionally, theorists with a background in mechanics use finite element calculations with stress/strain relations derived from triaxial tests. But some physicists claim that there is no proper definition of a displacement field in an object like a sand heap.

It will be argued that the crucial feature is the preparation history of the sample: some flowing sand settles and transforms into a frozen material. The distinction between flowing and frozen is sharp, and somewhat similar to a liquid solid transition. A flowing grain stops at a certain position X; later it moves with the frozen phase, by a certain amount u(X, t) and this defines a continuous displacement field.

An important notion is that of a correlation length ξ in the frozen phase. This may be related to the mesh size of the force network; and to the minimal size of slip bands. In typical systems, it is of the order 5 to 10 grain diameters. We argue that ξ is never very large in practical conditions: the fluid $\rightarrow$ frozen transition is the analogy of a first order transition. Many strange behaviors considered by the physicists are then eliminated.

Session: A1-2 Room: CUB 220 **Time:** M10:00a-12:00p
Chair: ***E. Samulski (U North Carolina)***

A Continuum Theory for Polymeric Liquid Crystals

Eringen, A.C.
Princeton University, USA

I shall present a continuum theory for liquid crystalline polymers involving the following notions:

- Flexible molecules
- Variable degree orientations
- Dissipation
- Electromagnetic interactions

Twisting Constraints in Conventional Polymers

Plewa, J. and Witten, T.A.
University of Chicago, USA

Though the backbone bonds of a hydrocarbon polymer are free to rotate in principle, there are strong kinetic barriers against the cis orientation. This barrier, if sufficiently high, would impose a conservation law on the polymer's motion. For example, a ring polymer would conserve its linking number as a DNA ring does. We report a lattice simulation that incorporates this constraint with a single backbone. The ratio of twist to writhe in these rings is much larger than for DNA chains. We sketch the consequences of the twist-storing constraint for the relaxation kinetics of linear, open polymers.

Structure and Dynamics of Block Copolymer Liquids

Lodge, T.
University of Minnesota, USA

Block copolymers comprise an important class of self-assembling macromolecular systems, that exhibit both lyotropic and thermotropic ordering phenomena. The length scales associated with these structures fall in the range 10-100 nm. And are amenable to study by small angle scattering (x-ray and neutron) and electron microscopy. The dynamics of these systems may be probed by rheological and light scattering techniques. Recent results from our laboratory will be presented, emphasizing styrene-isoprene copolymers.

Measures of Integration in the Statistical Mechanics of Polymers and Liquid Crystals

Helfrich, W.
Freie Universität, Germany

Usually it does not matter which measure of integration is chosen in the statistical mechanics of polymers, fluid membranes or liquid crystals. It may be a displacement, an angle or a curvature. However, there are situations where the choice does make a difference. We present a few examples of this type and discuss how the correct measure is derived from basic statistical mechanics in the classical case.

Session: A1-3 Room: CUB 220 **Time:** M1:30p-3:30p
Chair: ***T. Witten (U Chicago)***

Dynamic Surface Tension and Kinetics of Surfactant Adsorption at Fluid Interfaces

Andelman, D., Diamant, H. and Ariel, G.
Tel Aviv University, Israel

Surfactant kinetics at fluid-fluid interfaces is studied within a free energy formalism, which provides a general method for calculating dynamic surface tension. For non-ionic surfactants the results coincide with previous models. Common non-ionic surfactants are shown to undergo diffusion-limited adsorption, in agreement with experiments. On the other hand, ionic surfactants such as SDS without added salt behave quite differently. Strong electrolytes lead to kinetically limited adsorption, slower dynamics and intermediate plateau in the kinetic surface tension as was observed in experiments. Upon addition of salt the electrostatic interactions are screened and the adsorption becomes more similar to the non-ionic case. We also present results for the adsorption of a multi-component surfactant solution. We examine the case when one species has a fast diffusion in the bulk while the second species has a slower dynamics but a stronger affinity to the surface. At later times the competition results in the desorption of the faster species due to the adsorption of the surfactant with higher surface affinity.

Polymers and Liquid Crystals: The Parallel World of Computational Models

Windle, A.
University of Cambridge, United Kingdom

It is held in some quarters that the advent of computational modelling is changing the way we look at science. This statement will be explored in the context the application of different modelling approaches on different scales to polymers, liquid crystals and liquid crystalline polymers. Within the general hierarchy of time and distance, the presentation will focus especially on the so-called "meso modelling" and its sub-division at both nano and micro scales.

Ordered Phases of Block Copolymers and Lipids

Schick, M.
University of Washington, USA

Ordered phases of diblock copolymers have potential exciting application as templates for devices in nanotechnology. The role that the counterparts of these phases play in biological lipids is less clear, but equally fascinating. It is thought that they are important in processes in which the membrane requires regions of high curvature, such as excocytosis and membrane fusion. Recent advances in the theory of these phases in both block copolymer and lipid systems will be reviewed.

"Title to be Announced"
Chandrasekhar, S.

Similarities in Liquid Crystals and Entangled Polymers

Samulski, E.T.
University of North Carolina at Chapel Hill, USA

The local anisotropy present in the fluid phases of liquid crystals and polymer melts can have dynamically similar consequences: The local rotational diffusion incompletely averages second rank nuclear magnetic resonance interactions (e.g., quadrupolar and dipolar NMR interactions). Translational diffusion can eventually average these interactions to zero in cubic mesophases and quiescent polymeric fluids. We have recently demonstrated that it is possible to measure quite small proton dipolar interactions by the use of spin-echo experiments(1,2). We will illustrate the utility of the NMR experiments with studies of both isotropic polymer melts-showing how the slow, multi-chain processes (e.g., reptation) influence macromolecular dynamics-and anisotropic (sheared) melts. Our long-range goal is to couple NMR imaging with rheology in an effort to extract unique microscopic information from entangled melts subjected to shear.

1. P. T. Callaghan and E. T. Samulski, Macromolecules 30, 113 (1997).

2. R. C. Ball, P. T. Callaghan and E. T. Samulski, J. Chem. Phys. 106, 7352-62 (1997).

Session: A1-4 Room: CUB 220 **Time:** M4:00p-6:00p
Chair: ***D. Andelman (Tel Aviv U)***

Using Stochastic Simulations to Study the Dynamics of Polymer Melts and Liquid Crystals

Schieber, J.D.
Illinois Institute of Technology, USA

The dynamics of kinetic theory models for systems with microstructure are typically modeled by Fokker-Planck equations. Such equations do not usually yield much analytic information. However, stochastic simulations can provide an extremely powerful tool for studying these dynamics by exploiting the equivalence between Fokker-Planck equations and stochastic differential equations. Such simulations provide great insight into complex dynamics well into the nonlinear regime of flow dynamics. We consider here two recent simulation techniques developed with coworkers: an algorithm for studying Doi's model for liquid crystals, and a full-chain reptation model.

The first model scales linearly with ensemble size, instead of quadratically as do previous techniques.

Hence, we are now able to study ensemble sizes orders of magnitude larger, and without making consistent averaging approximations typical for such models. Our studies reveal a dynamics much richer than previously expected.

The reptation model allows self-consistent modeling of most important features of entangled polymer chain dynamics: chain stretching, chain-length fluctuations, constraint release, and chain retraction. We show that all features of shear flow can be well described well into the nonlinear regime, including the double-step-strain shearing flows of Osaki, *et al.*, of Venerus and Kahvand [*J. Polym. Sci*, **32**, 1531-1542 (1994); *J. Rheol.* **38**, 1297-1315 (1994)], and of Brown and Burghardt [*J. Rheol.* **40**, 37-54 (1996)].

Polymers, Liquid Crystals and Molecular Shuttles

Dennis, J., Howard, J. and Vogel, V.
University of Washington, USA

Nature has evolved specialized molecules, namely motor proteins, to actively transport molecules over long distances and against concentration gradients. Our goal is to develop molecular shuttles that can operate on surfaces under ex-vivo conditions. This includes creating nanoengineered surfaces across which molecular motors move materials, under user control, and between user-specified locations. We have used polymers to create surface textures that act as tracks for the movement of microtubules on kinesin functionalized surfaces. For a liquid crystal, which also is aligned on these surfaces, second harmonic generation gives insight on surface alignment mechanism.

Smectic a Liquid Crystals as Modulated Nematics: Phase Transition Studies

Calderer, C.
Pennsylvania State University, USA

Within the framework of mathematical modeling, we adopt the point of view that Smectic. A liquid crystal configurations are special periodic solutions of an *extended nematic* theory. In particular, we give an interpretation of the symmetry breaking phenomenon associated with the nematic—smectic. A phase transition, and derive the basic parameters that characterize a smectic. A phase in terms of those of the former nematic. We apply such ideas to the modeling of defects associated with the phase transition.

In the second part of the presentation, we discuss how the basic modeling features of such a transition are mathematically related to the mechanism responsible for texture and defects in certain polymeric liquid crystal flow. We conclude with the discussion of applications concerning the stability of liquid crystal droplets.

(Some of the topics presented here are joint work with Lev Truskinovsky, Bagisa Mukherjee and Chun Liu.)

Liquid Crystals and the Physics of Defects

Kleman, M.
Univ. Pierre et Marie Curie, France

Liquid crystals have offered a remarkable field of studies for the development of new concepts in the physics of defects. After a short introduction, stress will be put on new aspects in the topology and energetics of focal ionic domains, in particular, how their topology depends on the suddle-splay constant K_{23} in thermotropic SMA's and lyotropic lamellar phases.

Chiral Mesophases of DNA

Kamien, R.D.
University of Pennsylvania, USA

In the hexagonal columnar phase of chiral polymers a bias towards cholesteric twist competes with braiding along an average direction. When the chirality is strong, topological defects proliferate, leading to either a tilt grain boundary phase or a new "moiré state" with twisted bond order. This moiré phase can melt leading to a new phase: the chiral hexatic. I will discuss some recent experimental results from the NIH on DNA liquid crystals in the context of these theories.

Session: A1-5 Room: CUB 220 **Time:** T 9:30a-11:30a
Chair: ***W. Helfrich (Frei U Berlin)***

The Life and Death of "Bare" Viscous Bubbles

Debregeas G., and Brochard, F.
Institut P. et M. Curie, France

Air bubbles collect and explode at the surface of many viscous liquids, as observed with polymer foams, in glass furnaces, and during volcanic eruptions. The liquid film separating the bubble from bulk air can have a long lifetime (if it is viscous) even if it is not protected by a surfactant: these "bare" films display completely novel dynamic behavior in drainage and rupture. We studied this on two different model systems: a) a polymer melt (silicone oil), b) a molten glass of comparable viscosity. Although the two systems differ very much in their relaxation time, they are described by the same set of laws - which can be understood from a relatively simple hydrodynamic model.

Macroscopic Properties of Smectic C_G Liquid Crystals

Brand, H.
Universitat Bayreuth, Germany
Cladis, P.E.
Universitat Bayreuth, Germany, and Advanced Liquid Crystal Technologies, USA, and
Pleiner, H.
Max-Planck-Institut fur Polymerforschung, Germany

We discuss the macroscopic behavior of smectic C_G liquid crystals. The smectic C_G phase is the most general tilted smectic phase that is fluid in the layers. It is characterized by global C_1 symmetry. As a consequence, it is ferroelectric, pyroelectric and piezoelectric, opening up a number of possible applications for such a phase. Since the smectic C_G-phase has a macroscopic hand due to its structure, it can arise naturally in two enantionmorphs. Thus the smectic C_G phase appears as a natural candidate for the explanation of recent experimental observations of left and right-handed helixes in a system composed of a chiral molecules. We also discuss critically to what extent the smectic C_G phase might be important for the liquid crystalline phases formed by banana-shaped molecules. Phase transitions involving a smectic C_G phase and the defects of its in-plane director will also be briefly discussed.

Interfacial Correlations and Layer Undulations in Self-Assembling Liquid Crystalline Polymers

Shashidhar, R. and Geer, R.E.
Naval Research Laboratory, USA

Side chain siloxane liquid crystal polymers self-assemble into well ordered layers due to micropic scale phase separation between the siloxane backbone and the mesogenic side groups. This leads to a quenching of thermal fluctuations that are characteristic of smectic layers. As a consequence, self-assembled and highly ordered films of siloxane side chain polymers are convenient systems to study static undulations in layers of soft organic materials like polymers and liquid crystals. Results on the self-assembling nature of the layers, their structures and interfacial order are presented. It is also shown that the surface-induced static undulations penetrate deep into the interior of the film, in agreement with Professor de Genee's predictions in analogy with the London penetration depth in superconductors.

Liquid Single Crystal Elastomers (LSCE)

Finkelmann, H., Fischer, P., Stein, Peter and Stein, Pascal. Universität Freiburg, Germany

Liquid crystal elastomers can be macroscopically ordered with respect to the director by applying a mechanical field similar to electric/magnetic field orientation of low molar mass liquid crystals. Introducing network anisotropy a priori by the synthesis, uniformly aligned nematic or smectic elastomers are available without external mechanical field that combine optical properties of single crystals with entropy elasticity of elastomers.

Due to the uniform director orientation without defects, the LSCE's exhibit excellent transparency which makes them applicable for optical elements. Non linear optical properties can be easily optimized by attaching suitable l.c.-moities to the polymer network. On the other hand, due to the rubber elasticity of the LSCE, electro mechanical effects can be observed, e.g. piezo-electricity of elastomers. This concept can also be applied for polymer networks having discotic or amphiphilic monomer units.

Session: A1-6 Room: CUB 220 **Time:** T 1:00p-3:00p
Chair: *F. Brochard (Inst Pierre et Marie Cure)*

Thermomicropolar Flow of a Nematic Liquid Crystal in a Flexible Stenosed Tube

Narasimhan, M.N.L.
Oregon State University, USA

Flow of a thermomicropolar nematic liquid crystal in a flexible tube with a constriction is analyzed in this paper. The balance laws and constitutive equations along with the thermodynamic restrictions on material coefficients are presented for the nematic mesophase. The flexible tube wall is considered to be a linear elastic material given by an independent constitutive equation. Appropriate boundary conditions for the wall material and the fluid phase are formulated. The resulting field equations along with the boundary conditions are processed for solution and the physical implications are discussed.

Creating Functional Peptide Architectures At Interfaces

Tirrell, M., Fields, G., Yu, E., Ochsenhirt, S. and Pakalns, T.
University Of Minnesota, USA

Short peptide sequences, derived from whole proteins, can be useful synthetic agents for conferring a specific biological function to a material surface. Their ability to do this depends on delivering them to the surface in a biologically recognizable form, that is in a spatial configuration that is not too different from that adopted by the peptide in the whole protein. Most functional proteins have secondary and tertiary levels of structure that are essential to their activities; peptides have simpler but no less important structures. In our work, we have focussed on peptides derived from extracellular matrix proteins. We have found that attaching synthetic lipid tails to peptides fragments gives them two very useful properties for surface modification. The hydrophobic tails give rise to a self-assembly capacity enabling these molecules to

organize into membrane, monolayer and bilayer structures. Lee expected is that this level of self-assembly induces a second level in the peptide headgroup. Peptides from alpha-helical and triple-helical regions of protein are induced by the lipid tails to form protein-like secondary structures and therefore to have more effective biological activity.

"Title to be Announced"

Berker, N.

Session: A1-7 Room: CUB 220 **Time:** T 3:30p-5:30p
Chair: ***M. Kleman (U Pierre et Marie Curie)***

Brownian Motors in the Photoalignment of Liquid Crystals

Palffy-Muhoray, P.
Kent State University, USA

Since liquid crystals are soft anisotropic fluids, they can be aligned by light. The photoalignment of liquid crystals is of considerable current interest for display and other applications. The reorienting effect of light on nematic liquid crystals is greatly enhanced by the presence of a small amount of dissolved dichroic dye[1]. Irradiating photosensitive alignment layers with polarized light can also result in reorientation of the nematic director[2]. We show that the torque responsible for the reorientation is not the result of angular momentum transfer from the light, but occurs via an orientational ratchet mechanism, similar to the translational ratchet proposed by Prost[3]. The dye molecules act as rotors of a Brownian motor; the light field provides the energy which is dissipated in viscous shear. The results of simulations are compared with experiments, and novel aspects of the nonlinear optical response are discussed.

1. I. Janossy, Phys. Rev. E 49, 2957 (1994)
2. W. Gibbons, T. Kosa, P. Palffy-Muhoray, P.J. Shannon, S.T. Sun, Nature, 377, 43 (1995)
3. J. Prost, J.F. Chawin, L. Peliti, A. Ajdari, Phys. Rev. Lett. 72, 2652 (1994)

Microstructural Media in Bundle Space

Rymarz, C.
Military University of Technology, Poland

In this paper is the presentation the theory of differentiable manifolds is applied for modeling the deformation and kinematics in microstructural media. The microstructural material continuum is defined as a Cartesian product of the Euclidean E^3 and microstructural M spaces. The material, microstructural body $\mathbf{B}$ is the Cartesian product of proper subspaces of above differentiable manifolds; $\mathbf{B} = U \times M_1$ where $U \subset E^3$, $M_1 \subset M$. On the product of these manifolds, the bundle space Δ is constructed. The four following elements define its structure:

$$\Delta = (B, F, G, p)$$

where: *B- base space, F- fibre space, G – structural group, p- projection operator.* The base space $B \subset E^3$ is the classical material continuum, $F \subset M_1$. The structural group G depends on the kind of modeled microstructure. For micropolar medium G is the group of rotation and for the micromorphic one, the group of affine transformations. The projection operator p: $F \to B$ allows for continuous transition from microstructural to classical theory of continuous medium. The structural group G allows to define the geometry of the M space. In micropolar medium a metric tensor can be define in M (invariance of distance) and in consequence the Riemann affine geometry. In micromorphic medium only non-metrical geometry, with affine connection, can be defined. For determination of any rigid micro-body rotation three vectors (directors) should be known. In liquid crystals, due to high symmetry, only one director is taken into account. Hence any motion can be presented as a simple sum of vectors: $\mathbf{Z} = \mathbf{u} \oplus \mathbf{d}$, where $\mathbf{u}$ – displacement or velocity and $\mathbf{d}$ **– director.** Naturally $\mathbf{u}$ is defined in the tangent space of B and $\mathbf{d}$ in M. It doesn't concern differentials of these vectors, since the derivatives of values from the tangent space doesn't belong to it. It is a reason to define the mixed deformation measure in the form of the Cosserat tensor. To be free in order of superposition we define the symmetric Cosserat tensor. The second deformation measure should satisfy the compatibility conditions. It has the following form:

$$\Gamma^N_{KM} = Q^{mN}_{,K} Q_{mM}$$

Its anti-symmetric parts is very known wryness tensor.

I hope that some preliminary considerations on micromorphic media will be presented during my lecture.

Liquid Crystals. From Synthetic Goal to Synthetic Tool

Percec, V.
Western Reserve University, USA

This lecture will describe the evolution of the research on molecular, macromolecular and supramolecular liquid crystals (LCs) in our laboratory. Particular examples that will demonstrate the evolution of this research originally aimed to LC molecules with extremely simple architecture to molecules and macromolecules with complex architecture and subsequently the transition of this research from LCs as a synthetic goal to LCs as one of the most efficient synthetic tools for the retrosynthetic analysis and design of supramolecular synthons used in the construction of supramolecular giant soft systems[1-9] will be presented.

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Wavelength Doubling Cascade to Möbius Defect Turbulence in a Nematic Liquid Crystal

Fradin, C.[1,2], *Brand, H.R.*,[3,1] *Finn, P.L.*[1,4] *and Cladis, P.E.*[1,3,4]
[1]*AT&T Bell Laboratories, USA*
[2]*Service de Physique de l'État Condensé, France*
[3]*Universität Bayreuth, Germany*
[4]*Advanced Liquid Crystal Technologies, USA*

The following wavelength doubling cascade from a uniform state to a turbulent pattern is observed in a nematic liquid crystal: first oscillating convective rolls followed by a stationary stripe pattern, then Möbius defect creation stabilizing an unusual curved roll pattern that eventually becomes turbulent. Once created, Möbius defects are topologically trapped and the initial uniform state is not recovered. The system experimentally investigated is electroconvection above a highly nonlinear base state.

Session: A1-8 Room: CUB 220 **Time:** W 9:30a-11:30a
Chair: ***S. Chandrasekhar (Center of Liquid Crystal)***

Some Recent Mathematical Approaches to the Theory of Liquid Crystals

Liu, C.
Pennsylvania State University, USA

In the last twenty years, there has been much work on the mathematical analysis of the modeling of the liquid crystal materials. For instance, the understanding of the defect configurations by minimizing the Oseen-Frank energy is connected to the study of the harmonic maps, the droplets are related to the free boundary problems, and the structure of smectic. A can be treated as Dupin Cyclides and in some cases related to the Willmore conjecture. These applications also motivated many developments in the theory of calculus of variations and partial differential equations. In this talk, we will explore some of these connections. We will look at a new free energy which was introduced by Calderer and Palffy-Muhoray in order to study the phase transition between smectic A and other phases. Finally, we will discuss some different dynamic systems and study the influence between the flow velocity and the defect configurations.

(Some of the topics discussed here are joint work with Carme Calderer, David Kinderlehrer, Fanghua Lin and Noel Walkington.)

Interactions of Liquid Crystals with Physical Fields in Variational Description

Kotowski, R. and Radzikowska, E.
Polish Academy of Sciences, Poland

Since that time when the papers of the Cosserat brothers have been published the practical importance of materials with inner degrees of freedom has been proved by technological developments. The theories of media with inner degrees of freedom were the first generalizations of pure local continuum theories where structureless material points are considered only. In polar theories material points are treated as rigid particles (in micropolar media) or as deformable particles (in micromorphic media). The new degrees of freedom are described either by rigid or deformable directors attached to geometrical points. In the simplest case, as for example in the theory of nematic liquid crystals, only one rigid director is assumed. We adopt the kinematics of micropolar media from the papers of Eringen and Eringen and Kafadar.

We construct a variational theory of micropolar media which is able to describe both reversible and irreversible processes. We were inspired by the famous article of Natanson from 1896 and the methodology proposed by Sedov.

The variational principle as discussed in the present paper is a generalization of the Grot variational principle. The generalization concerns the microstructure of the medium and thermodynamic interactions.

The basic balance laws obtained from the postulated variational principle together with those assumed in our variational approach and supplemented by the constitutive relations, compose the complete system of equations describing liquid crystals interacting with electromagnetic, mechanical and temperature fields. Our variational approach includes both the thermodynamically equilibrium and the nonequilibrium states of liquid crystals, since the dissipative processes are taken into consideration.

The variational principle proposed in the paper for the simple micropolar medium has an universal form and can be applied to the description of the other types of continuous media interacting with external fields. Liquid crystals were chosen to exemplify our method

because of their great practical importance. The fundamental definitions and theorems of the variational calculus are formulated. The polynomial nonequilibrium constitutive equations of nematic liquid crystals obtained from the constitutive equations theory are presented in the Lagrangian description.

Remarks About the Dynamics of the Fokker-Planck Equation

Kinderlehrer, D.
Carnegie Mellon University, USA

Nonlinear systems which are active across disparate length and time scales are among the most intriguing ones we encounter in nature. Moreover, many of these systems, although persistent for long times, reside in metastable states and their evolution is poorly understood. We are, thus, presented with difficult scientific challenges, both in the derivation of appropriate frameworks for modeling and in the effective use of large scale simulation techniques for their execution. We focus here on a mechanism we believe to be deeply intertwined with these properties. This is the competition between the thermodynamic energy and nearness in the appropriate sense for the distribution of microscopic variables, the 'averages' that describe the evolution of the macroscopic system. The result is a new derivation of the Fokker-Planck Equation as the gradient flux or steepest descent of the ordinary thermodynamic energy (e.g., minus the entropy in the case of ordinary diffusion or Brownian motion). When the role of the entropy is small, we may apply these notions to analyze hysteresis in shape-memory systems. We would like to investigate Brownian rachets, a situation where fluctuations are prominent.

This is joint work with Richard Jordan and Felix Otto.

Symposium A2

Constitutive Models and Penetration Mechanics. In honor of the 1998 SES Medalist Professor Sol Bodner

Organizers

K. S. Chan & C. Anderson
Southwest Research Institute. USA

Session: A2-1 Room: Auditorium **Time:** T8:00a-9:00a
Chair: ***C. Anderson (Southwest Research Institute)***

The Art of Formulating Elastic-Viscoplastic Constitutive Equations

Bodner, S.R.
Israel Institute of Technology, Israel

Despite the intention to be scientific, the formulation of elastic-viscoplastic constitutive equations is somewhat of an art form. The reason is that the mechanisms of inelastic deformation are exceedingly complex and judgment has to be exercised between the desired simplicity of the equations and the need to adequately represent the relevant physical response characteristics over the range of loading conditions, strain rates and temperatures of interest. This paper discusses some of the factors involved in the development and application of such constitutive equations, namely: the extent to which the physics of the deformation processes can be included in the equations, the mechanical and thermodynamical restrictions, the associated test program for the determination of the material parameters, and the process of obtaining the parameters from the test data - the parameter identification problem. These factors are necessarily coupled and could be expected to lead to alternative formulations for different materials and conditions. Examples of elastic-viscoplastic constitutive equations for various materials, namely, some metals, rock salt, and excised facial skin, will be discussed.

Session: A2-2 Room: CUB214-16**Time:** M10:00a-12:00p
Chair: ***C. Anderson (Southwest Research Institute)***

Viscoplasticity at Static and Dynamic Loading Rates

Krempl, E. and Sham, T.L.
Rensselaer Polytechnic Institute, USA

In the static regime, say below 10^{-2} 1/s rate independent plasticity is generally used for modeling the inelastic deformation behavior of engineering alloys at ambient temperature. In the dynamic range from approximately 10^{-2} to 10^{7} 1/s, viscoplastic models are in use. In the slow dynamic region the flow stress at a given strain increases in the order of several percents for every decade change in strain rate. At very fast strain rates, between 10^{4} to 10^{7} 1/s, the flow stress dependence on strain rate can be almost linear. It is also reported that stress-strain curves obtained at various strain rates in the slow dynamic regime of fcc metals and alloys tend to diverge whereas those of bcc metals and alloys are nearly equidistant when inelastic flow is fully established. Quasi static experiments with servo-controlled testing machines on ductile metals and alloys show changes of the flow stress with strain rate comparable to those found in the slow dynamic regime. It appears that viscoplastic behavior is exhibited over the entire strain rate spectrum from, say, 10^{-6} to 10^{7} 1/s and that viscoplastic models are therefore appropriate. The viscoplasticity theory based on overstress (VBO) can be applied to this wide strain rate spectrum. VBO is a "unified' state variable theory where the inelastic rate of deformation is an increasing function of the overstress (effective stress), the difference between the stress and the equilibrium (back) stress. The drag stress can be introduced as an additional state variable. It is shown that the response of VBO for a given strain rate is bracketed on the one hand by a linear response with a slope equal to the elastic modulus for infinite strain rate. The slow response for vanishing strain rate, on the other hand, is traced out by the equilibrium stress-strain curve. Hardening can either be modeled by a growth of the equilibrium stress and/or of the drag stress. Pure equilibrium stress hardening makes the hardening rate-independent and produces ultimately equidistant stress-strain curves resembling those of bcc metals and alloys. A drag stress increase causes viscous hardening and renders stress-strain curves similar to those of fcc metals and alloys. These properties are demonstrated by numerical experiments in the strain rate range from 10^{-6} to 10^{6} 1/s using one set of material constants.

A Model for Predicting Grain Boundary Cracking in Multi-Grain Crystalline Viscoplastic Materials

Allen, D.H., Helms, K.L.E.
Texas A&M University, USA, and
Hurtado, L.D.
Sandia National Laboratories, USA

Crystalline materials such as metals experience a variety of inelastic and therefore thermodynamically dissipative processes during deformation. These may include several types of dislocation rearrangement mechanisms within grains, as well as fracture and/or sliding along grain boundaries. When these processes occur at temperatures that are generally in excess of about three tenths of the melting point of the solid, they are inherently rate dependent. Due to the complexity of these events, and the fact that they occur in multiple grains simultaneously, analytic models of these phenomena have not been completely developed at this time.

One part of this problem that is quite difficult deals with the dissipative processes that occur along grain boundaries. Due to the migration of dislocations to grain boundaries, vacancies can open up, thereby assisting sliding and fracture between grains. In some environmental circumstances this process can produce the majority of energy dissipation during loading. Thus, models that can physically account for this mechanism are needed.

In the current paper, the author will discuss the deployment of a rate dependent cohesive zone model to account for the process of grain boundary fracture and/or sliding. This will be formulated within the framework of the finite element method, and inelasticity within the grains will be accounted for by employing a viscoplasticity model of the Bodner-Partom type. Examples will be given for a multi-grain solid subjected to boundary tractions that lead to grain boundary fracture induced by dislocation pileups at grain boundaries.

Propensity for Spall Formation in Salt Storage Caverns Using a Creep and Fracture Analysis*

Munson, D.E
*Sandia National Laboratories**, USA*

There are a relatively large number of hydrocarbon, gaseous and liquid, as well as basic feed stock, storage caverns in the U.S. These storage caverns are often constructed in massive salt deposits by dissolutioning of the salt. Immense caverns with capacities of millions of barrels are formed this way. In storage caverns, liquids are normally transfer by brine displacement through very long, often several thousand feet, hanging strings of casing. Many well documented hanging string events have occurred in the storage caverns of the Strategic Petroleum Reserve (SPR) in the Gulf Coast salt domes, suggesting impact damage and loss of casing in many instances is the probable result of salt spalls falling in the cavern. Indirect evaluation of the cavern conditions indicate that the greatest occurrence of damage is associated with those caverns with very large rates of accumulation of salt material, presumably from salt falls. The salt certainly comes from the sides of the cavern and is primarily masses that are too small to cause damage. Only a few of the salt spalls are sufficiently massive to damage the hanging casing, and only a few actually hit the casing string. While the salt falls are thought to cause the damage, the propensity for these falls varies markedly between the storage facilities in the different salt domes, and also within the caverns of a given dome. In an attempt to explain these differences, it was necessary to look for a fundamental model of salt fall formation. The Multimechanism Deformation Coupled Creep (MDCF) [1] model of creep and fracture is believed to offer the proper type of response. One aspect of the model is that the amount of time dependent material damage is strongly related to impurity content of the salt, which potentially explains the marked variation between the different dome sites, and the caverns in a given dome. The impurities in a salt dome are non-uniformly distributed, with relatively local concentrations. Impurity levels of the domes also differ. Using this as a basis, a series of calculations were performed using a finite element code and the MDCF model. Smooth wall caverns, under typical cavern geometries and operation conditions show little material damage. It is necessary to have protrusions and irregularities of the cavern wall to produce sufficient damage, and potential spall features. Two cases of idealized protrusions are examined, which produce the conditions for spall.

[1] Chan, K. S., D. E. Munson, A. F. Fossum, and S. R. Bodner, Int'l. J. Damage Mech., 5, 125-140, 1996.

*Work supported by U. S. DOE under contract DE-AC94-A185000
**A DOE facility, operated by Sandia National Laboratories division of Lockheed Martin

Application of Isochronous Healing Curves to Predicting Damage Evolution in a Salt Structure*

Chan, K.S., and Bodner, S.R.,
Southwest Research Institute, USA, and Munson, D.E.
*Sandia National Laboratories**, USA*

A treatment of damage healing formulated within the framework of continuum damage mechanics is presented for rock salt. The concept of an isochronous healing surface, which is a locus of points in a stress space for which times of healing are identical, is proposed and derived from the healing formulation. The characteristics of the isochronous healing curve are identified and compared against those of an isochronous failure curve and the dilatancy boundary. Isochronous healing curves for clean and argillaceous (containing clay particles) salt are developed and evaluated against laboratory data. Subsequently, the isochronous healing curves are used to predict the healing response of damage in the disturbed rock zone of an air intake shaft in a salt structure.

*Work supported by U. S. DOE under contract DE-AC94-A185000
**A DOE facility, operated by Sandia National Laboratories division of Lockheed Martin

Session: A2-3 Room: CUB 214-16 **Time:** M1:30p-3:30p
Chair: *R. C. Batra (VPI)*

Shear Band Spacing in Dipolar Thermoviscoplastic Materials

Batra, R.C., and Chen, L.
Virginia Polytechnic Institute and State University, USA

We study thermomechanical deformations of a rigid viscoplastic body deformed in simple shear. The strain gradients are taken as independent kinematic variables and the corresponding higher order stresses are included in the balance laws and the constitutive relation. Two different functional relationships, the power law and that proposed by Wright and Batra, are used to relate the effective strain rate to the effective stress and temperature. Effects of strain hardening of the material are neglected. The homogeneous solution of the problem is perturbed and the stability of the equations linear in the perturbation variables is studied. Following Wright and Ockendon's postulate that the wavelength of the dominant mode determines the minimum spacing between adjacent shear bands, the shear band spacing is computed. It is found that the shear band spacing is sensitive to the thermal softening, the material characteristic length and the nominal strain rate. Approximate analytical expressions for the shear band spacing are also derived.

Penetration of 6061-T6511 Aluminum Targets by Ogive-Nose Steel Projectiles With Striking Velocities Between 0.5 and 3.0 Km/s

Warren, T.L.. Sandia National Lab, USA
Piekutowski, A.J., University of Dayton Research Institute, USA
Forrestal, M.J., Sandia National Lab, USA
Poormon, K.L., University of Dayton Research Institute, USA

We performed a series of depth-of-penetration experiments using 7.11-mm-diameter, 71.12-mm-long, ogive-nose steel projectiles and 254-mm-diameter, 6061-T6511 aluminum targets. The projectiles were made from VAR 4340 (R_C 38) and AerMet 100, (R_C 53) steel, had a nominal mass of 0.021 kg, and were launched using a powder gun or two-stage, light gas guns to striking velocities between 0.5 and 3.0 km/s. Since the tensile yield strength of AerMet 100, R_C 53 steel is about 1.5 times greater than VAR 4340, R_C 38 steel, we were able to demonstrate the effect of projectile strength on ballistic performance. Post-test radiographs of the targets showed three different regions of penetrator response as striking velocity increased: (1) the projectiles remained visibly undeformed or rigid; (2) the projectiles deformed, without nose erosion, during penetration and deviated from the target centerline, exiting the side of the target, or turning severely within the target; and (3) the projectiles eroded during penetration and lost mass. To show the effect of projectile strength, we present depth of penetration versus striking velocity data for both types of steel projectiles at striking velocities ranging from 0.5 and 3.0 km/s. In addition, we show good agreement between a cavity-expansion model and the rigid-projectile penetration data.

Acknowledgment-This work was supported by the United States Department of Energy and the Joint DOD/DOE Munitions Technology Development Program.

Use of Bodner-Partom Constitutive Model to Describe High Strain Rate and Shock Response of Several Metals

Rajendran, A.M.
Army Research Laboratory, USA

The Bodner-Partom (BP) viscoplastic equations were used to accurately describe the high strain rate and shock response of several metals, such as OFHC copper, HY100, AF1410, C1008, and 1020 steels, and several aluminum alloys. The effects of strain rate and temperature on the strain rate sensitivity of OFHC copper were modeled using modified versions of the BP model. These modeling exercises were performed with reasonable success and without any extensive modifications to the original equations. A suite of stress-strain curves at elevated temperatures as well as at extremely high strain rates were successfully reproduced using the BP model. In addition, the mathematical form of the BP equations provided an elegant way to couple the viscoplastic behavior of the matrix material to void nucleation and growth in the aggregate material. The BP and void growth equations were implemented in a shock-wave-based finite element code called EPIC and several plate impact (shock wave) experiments were simulated.

This combined BP and void growth model successfully predicted the evolution of spall in various metals.

On the Hydrodynamic Approximation for Long-Rod Penetration

Anderson, C.E., Jr. and Walker, J.D.
Southwest Research Institute, USA, and
Orphal, D.L., and Franzen, R.R.
International Research Associates, USA

Steady-state hydrodynamic theory, or variations thereof, have been applied to long-rod penetration since the 1940's. It is generally believed that projectile strength is of little consequence at high velocities, and that hydrodynamic theory is applicable to long-rod penetration when penetration pressures are much greater than the target flow stress. Substantiating this belief is the observation that at approximately 2.5 km/s,

for tungsten alloy projectiles into armor steel, normalized penetration (P/L) nominally saturates to the classical hydrodynamic limit of the square root of the ratio of the projectile to target densities. We have experimental data, however, that show penetration velocities and instantaneous penetration efficiencies fall below that expected from hydrodynamic theory, even at impact velocities as high as 4.0 km/s. Numerical simulations, using appropriate strength values, are in excellent agreement with the experimental data. Parametric studies demonstrate that both projectile and target strength have a measurable effect even at such high impact velocities.

Session: A2-4 Room: CUB 214-16 **Time:** M4:00p-6:00p
Chair: ***K. S. Chan (Southwest Research Institute)***

Fracture of Yawed Rods that Penetrate Finite Plates

Bless, S.J., and Satapathy, S.
Institute for Advanced Technology, USA

Yawed rods that penetrate oblique plates experience erosion, deflection, deformation, and fracture. Experiments conducted in the reverse ballistic mode with tungsten rods striking RHA plates at 2.2 to 3.0 km/s provide a data set for evaluation kinematic and material response. Modeling of transverse motion in rods is based on the concept that plane-strain cavity expansion forces in the target are balanced by centrifugal forces in the rod. Forces are non-uniform due to the evolution in slot geometry and variations in confinement associated with plate obliquity. Fracture criteria are derived from dynamic bending tests. Agreement between the model for deflection and deformation and experiments is demonstrated. Fracture criteria require additional calibration from the experiments.

Response Sensitivities, Parameter Estimation, and the Bodner-Partom Equations

Fossum, A.F.
Sandia National Laboratories, USA, and
Senseny, P.E.
Factory Mutual Research Corp. USA.

Sensitivities of stress to parameter variations for the Bodner-Partom constitutive law are determined for a cyclic ratcheting test performed on a nickel-base superalloy at a high temperature (1093° C) to assess the utility of this test to determine a complete set of material parameters for the Bodner-Partom equations. The test comprises a series of ratcheted stress-strain hysteresis loops conducted in strain-rate control until saturation is reached. Each loop is defined by a ratcheting sequence in which a constant strain-rate is imposed followed by a dwell, i.e., a pure relaxation. Most of the stress induced during the constant strain-rate segment relaxes during the dwell. This sequence is repeated until a complete hysteresis loop is mapped out, first by ratcheting in tension and then by ratcheting in compression. The entire loop is then repeated until saturation, i.e., a stable hysteresis loop, is reached. The stress sensitivities are determined by differentiating the stress with respect to each constitutive parameter and are plotted over the entire loading history. This plot shows the sensitivity of the stress response to changes in each of the material parameters over the complete load path. Thus a graphical representation is available as an aid in assessing the utility of the test, i.e., whether or not the test provides enough information, indicated by significant sensitivity, to estimate each parameter. The ideal situation is one in which the sensitivity coefficient of each parameter is significantly higher than that of other parameters for a part of the test, or at least is one of the high sensitivity coefficients so that the parameter's contribution to material behavior can be determined. The stress sensitivities are also used in a gradient-driven optimization scheme to evaluate a well-determined parameter set. The classical method of parameter estimation for the Bodner-Partom Equations is used to determine the initial parameter estimates from test data. By using the optimization procedure combined with the calculated response sensitivities, not only can the initial parameter estimates be improved by getting a better fit to the data, but also, confidence intervals can be determined for the parameters as well as the correlation among the parameters.

Nontraditional Striker Impact

Goldsmith, W.
University of California-Berkeley, USA

More than 95% of published investigations involving projectile collisions can be classified as "standard", defined as the orthogonal impact of purely translating strikers on stationary solid targets; non-standard impacts are all other cases that invariably occur in the field in one form or another. Impingement of projectiles has been studied since the 1700's; for the first 150 years, only empirical results were obtained. Since about 1890, semi-empirical and quasi-rational approaches have been developed. This century has seen the enormous growth of phenomenological modeling, computational analysis—which provides for both spatial and temporal discretization and relies on material behavior description, including failure—and extended test methodologies due to the vast improvement of observation and measuring devices. Basically, whether standard or otherwise, impingement of a striker on a target can result in embedment, perforation or ricochet.

Penetrators are defined as objects with at least one axis of symmetry: they are classified here as spheres, projectiles with a length to diameter or aspect ratio (L/D) < 5 and long rods where L/D > 10; the domain between 5 < L/D < 10 can be classified either way. A

critical characteristic of a target is its thickness which frequently governs the damage phenomenon upon impact: thin targets are those with a thickness h/D < ½ or 1, where the stress and strain distribution in the thickness direction is uniform; intermediate thicknesses are those targets where 1 < h/D < 5, and the effect of the distal surface plays a noticeable role; and thick or semi-infinite targets, h/D > 10 where the presence of the distal surface can be neglected.

Major areas of non-standard impact include obliquity, yaw, yaw and obliquity, moving targets, striker spin, tumbling projectiles, and ricochet. Impact can occur in the subballistic range, with initial velocity v_o < 500 m/s; the ballistic or ordnance range, 500 < v_o < 1500 m/s; the ultra-ordnance range, 1.5 < v_o < 3 km/s, and the hypervelocity range, v_o > 3 km/s; all limits are approximate.

Characterization of the various types of non-standard conditions is categorized by type of striker (sphere, projectile, rod), by velocity regime, and by methods of investigation: analytical and experimental; experimental and numerical; experimental, analytical and numerical; or each of these categories by itself. Target damage can occur by indentation or penetration as well as scabbing, bulk deformation of the target element, fragmentation and fracture; perforation which may also include plugging, hole enlargement, scabbing, petalling, and bulging. Further, composites may experience delamination and fiber failure, while brittle substances, such as ceramics may exhibit comminution.

Some results involving non-standard impact will be briefly presented with concentration on cases involving correlation of test data with predictions.

Techniques for Measurement and Constitutive Modeling of Dynamic Deformation

Khan, A.S.
University of Maryland- Baltimore County, USA

Plate impact, split-Hopkinson-bar and direct disc impact techniques for measuring dynamic deformation will be critically reviewed and existing experimental data from each technique will be compared and discussed. Some of the leading constitutive models, e.g. Bodner-Partom, Johnson-Cook & Zerilli-Armstrong, will be discussed. Old and new results on 1100-0 Aluminum, OFHC Copper, tantalum and tantalum alloys, and titanium will be presented and compared with predictions from these models. A version of each model, with same number of material constants, will be selected for comparison. The selected experimental data will be over a wide range of strain-rate and temperature.

Symposium A3
Prager Medal Symposium. In honor of the 1998 Prager Medalist Prof. John R. Willis.
Organizer
P. P. Castaneda,
University of Pennsylvania, USA

Session: A3-1 Room: Auditorium **Time:** W8:00a-9:00a
Chair: ***P. P. Castaneda (Pennsylvania)***

Progress and Prospects for the Analysis of Nonlinear Composites.

Willis, J.
Cambridge University, United Kingdom

Up to the mid-1980's the only analyses of nonlinear composite response were based on the study of stress or strain increments coupled with use of ad hoc approximations. Around that time, it was recognized that, at least for response that could be described in terms of a convex potential function (such as deformation theory of plasticity, or steady-state creep), associated variational principles could be exploited to develop rigorous bounds for the corresponding overall potential. Such bounds are useful in their own right and, at the very least, provide a partial check on the validity of ad hoc approximations of possibly wider applicability. The first such development was the introduction of a comparison medium and an associated variational structure of Hashin-Shtrikman type. Choice of a linear, uniform, comparison medium then provided bounds for nonlinear problems which were direct analogues of the Hashin-Shtrikman bounds for linear composites. These bounds took account of the two-point statistics of the composite. The next development, due to Ponte Castaneda at the end of the eighties, was to introduce a comparison linear composite. In its original form this made direct use of any known bound for the linear composite, coupled with an optimization over its defining parameters. It allowed the introduction of more statistics but could fail in pathological cases. This problem was later removed (by Talbot and Willis) by combining the use of a comparison composite with the Hashin-Shtrikman technology.

A fundamental limitation was the use of a linear comparison medium. This allowed the construction of only one bound—either a lower bound or an upper bound—and, in certain cases, no bound at all. Quite recently, nonlinear comparison media have been used. These allow the construction of upper and lower bounds, always, but at the expense of introducing relatively sophisticated analysis.

This is, essentially, where rigorous theory is, to date. Progress is nevertheless being made. For example, a new scheme of "self-consistent" type has been devised by Ponte Castaneda. So far, it appears never to violate bounds, in contrast to all previous such schemes. Perhaps it can be developed further. In any case, it has been demonstrated to follow from a variational principle.

A separate development is concerned with fields that vary too rapidly for ordinary "effective modulus" theory to apply. A variationally based nonlocal theory has been formulated and is in process of being worked out in detail. Finite deformations provide a challenge: almost nothing is known rigorously. Even good approximations are not in evidence, though perhaps something may soon emerge. The lecture will allude, at least briefly, to all of these developments, and explain in more detail the recent ones, including any that may have become clarified between the time of writing and the time of the conference.

Session: A3-2 Room: Cascade 127 **Time:** T9:30a-11:30a
Chair: *R. Luciano (U. Cassino) &*
P.M. Suquet (LMA/CNRS)

Higher-Order Micromechanics-Based Nonlocal Constitutive Models for Elastic Composites

Drugan, W.J.
University of Wisconsin-Madison, USA

A generalization of the Hashin-Shtrikman variational formulation to random composites, due to J. R. Willis, is employed to derive a micromechanics-based, explicit nonlocal constitutive equation relating the ensemble averages (or volume averages) of stress and strain for a class of random linear elastic composite materials. The analysis builds on that of Drugan and Willis (1996, Journal of the Mechanics and Physics of Solids, Vol. 44, pp. 497-524), who analyzed two-phase composites with any isotropic and statistically uniform distribution of phases (which themselves may have arbitrary shape and anisotropy) and showed that the leading-order correction to a macroscopically homogeneous constitutive equation is a term proportional to the second gradient of the ensemble average of strain. Here I show that the next nonlocal correction term for such composites is proportional to the fourth gradient of average strain, and I derive completely explicit results for the case also explicitly analyzed by Drugan and Willis: composites consisting of an isotropic matrix reinforced/weakened by a random distribution of isotropic, non-overlapping identical spheres. Thus, this new result provides an accurate nonlocal constitutive equation valid down to very small volume size scales and to rather strong variations of average strain with position. Among several applications to be illustrated, it affords an analytical assessment of the size scale over which a leading-order nonlocal constitutive equation like that derived by Drugan and Willis would be expected to be applicable. It also permits accurate assessment of the remarkably small predictions derived by Drugan and Willis of the minimum representative volume element

size needed for accuracy of the standard constant-effective-modulus macroscopic constitutive equation for elastic composites.

Non Local Constitutive Relations for Heterogeneous Materials

Luciano, R.
University of Cassino, Italy and
Willis, J.R.
Cambridge University, United Kingdom

The static and dynamic analysis of structures realized in composite materials is extremely difficult if all the heterogeneties of the material are taken into account. An efficient tool to approach the problem is to estimate the overall elastic properties of the composite by using homogenization techniques and, then, to study the structure considered as homogeneous. In many cases the non-linear overall behaviour of the composite is characterized by a softening branch which makes the elasto-static or elasto-dynamic problem ill posed and leads to strain localization. Non local constitutive relations are efficient strain localization limiters and a means to preserve well-posedness of non linear elastic boundary value problem in presence of material softening behaviour. It is possible to deduce non local constitutive laws by using a phenomenological or a micro-mechanical approach. Micro-mechanical constitutive laws can be derived by following two hypotheses: the microstructure of the material is periodic or random. The first hypothesis has been adopted in order to obtain a non local constitutive equation by using the asymptotic method of homogenization. The second hypothesis has been used (Drugan, W. J. and Willis, J. R., *1996, J. Mech. Phys. Solids 44, 497*) to present an explicit constitutive equation which relates the mean strain with the mean stress. In this paper a non local constitutive model is presented for heterogeneous materials subject to microscopic and macroscopic body forces. A relationship between the ensemble average of the stress and of the strain is formulated in the Fourier and the space domain. Finally, it is explained how to treat the periodic heterogeneous materials as random materials and several examples are presented.

Helical Inclusion in an Elastic Matrix

Slepyan, L.I., Krylov, V.I., and Parnes, R.,
Tel Aviv University, Israel

Elastic space containing an elastic helical rod is considered. Uniform axial and radial extension and torsion of the composite are studied. Besides, internal torsion of the inclusion, aligned into a smooth helical canal in the elastic matrix, is examined as well. In a helix-associated coordinate system, due to translation-rotation helical symmetry, stress-strain fields are two-dimensional: they are uniform respective to the helical coordinate. Along with the helical symmetry, reflection symmetry is assumed. Under these conditions, only radial, distributed along the rod, inclusion-matrix interaction forces and moments exist, and the rod has only radial displacements relatively the global deformation of the matrix. Stress-strain and displacement fields in the matrix are represented by way of superposition of fundamental solutions corresponding to the homogeneous elastic space under a concentrated force and a concentrated moment. Two densities of these auxiliary singularities are the main unknowns. In terms of these densities, radial forces and moments acting on the rod and its radial displacements are calculated based on the fields in the matrix on the prospective interface. The two unknowns are then obtained from the condition that the rod radial displacement, its elongation, bending and torsion have to satisfy the corresponding nonlinear equations. In this way, the internal forces and moments in the rod as well as the displacement and stress-strain fields in the matrix are derived.

Along with the exact results, asymptotic solutions of two kinds are presented. The first one corresponds to a condition when curvature of the helix, K is small and the angle between the helix and its axis, α, is not too close to $\pi/2$. Namely, this asymptote is valid when $k_p << \cos\alpha$, where f is the rod cross-section radius. This allows the interaction forces and moments to be analytically determined based on the fields in the matrix. The second asymptote corresponds to a long-pitch helix, when the angle α and the helix radius tend to zero in such a way that $k \to 0$, but torsion of the helical rod axis $t \to$ const # 0. This means that the helix becomes a straight line, but the normal forms a screw surface like in the case of a `genuine' helix. In this case, the whole of the solution is derived analytically.

Microstructure Evolution in Voided Nonlinear Materials

Garajeu, M., and Suquet, P.M.
L.M.A./C.N.R.S., France

Fracture of ductile materials is governed by microscopic mechanisms which are well identified. First, voids are nucleated at precipitates or hard inclusions. In a second stage, these voids grow by plastic deformation of the matrix material surrounding them. In the third and last stage, some voids coalesce and form a macro defect which eventually leads to the final fracture of the structure. The present study is devoted to a model for the growth of voids in viscous nonlinear materials up to coalescence. The emphasis is put on the change in shape and distribution of the voids under axisymmetric loadings. An estimate for the potential of materials containing ellipsoidal voids is derived and used to account for the change in shape of the voids. The distribution of voids also evolves with the deformation of the material and large areas of matrix take place between the voids. Following Gologanu *et al.* (1994) the formation of these matrix-

rich zones is taken into account by an elementary model in which the voided material is seen as a lamination of the unvoided matrix together with porous layers. In the porous layers the voids are ellipsoidal and evolve in shape. The proposed model contains three damage parameters, the void volume fraction, the voids aspect ratio and the distribution aspect ratio as initially proposed by Kailasam, Ponte Castañeda and Willis (1997).

The predictions of the model are compared with numerical simulations by FEM of the deformation of voids in a viscous matrix. The evolution of the overall strain and the porosity are correctly picked up. In particular the rapid changes in porosity at incipience of coalescence are well predicted. M.

Gologanu, J.B. Leblond and J. Devaux: *Computational Material Modeling*, ASME Pub. AD **42**/PVP- **294**, 223-244, 1994.

M. Garajeu: *C. R. Acad. Sci. Paris*, **323** Série II b:307--314, 1996.

M. Kailasam, P. Ponte Castañeda, and J.R. Willis: *Phil. Trans. R. Soc. Lond. A*, **355**:1835--1852, 1997.

Session: A3-3 Room: Cascade 127 **Time:** T1:00p-3:00p
Chairs: *G.W. Milton (U. Utah) &*
P. P. Castaneda (Pennsylvania)

Bounds on the Stress-Strain Relation for Non-Linear Composites

Milton, G.W.,
The University of Utah, USA

Considerable work has been done on bounding the elastic energy of non-linear composites. Yet the stored elastic energy is a difficult quantity to measure, requiring one to integrate the work done to achieve a given deformation. From a practical viewpoint it may prove more important to bound the average stress given an average strain since these are direct physically measurable quantities. In this lecture we show how this can be done, using some new variational principles for non-linear elasticity. These variational principles are the natural generalization to non-linear problems of the variational principles Cherkaev and Gibiansky obtained for linear viscoelasticity. The problem is reduced to bounding a certain function and the same methods that have been developed to bounding energies can be directly applied to bounding this function.

Two-Dimensional Composites: Advances in Linear and Nonlinear Conductivity

Nesi, V., Universita degli Studi di Roma La Sapienza, Italy

We consider a two-dimensional conducting medium. We present first optimal bounds for the effective conductivity in linear problems. These results use methods which are different both from the Hashin-Shtrikman and from the compensated compactness (translation) method. Then we present various applications to related (power law) non linear problems when the nonlinearity is superquadratic. These include improved new lower bounds for three-phase materials (joint work with D. R. S. Talbot and J. R. Willis) and new upper bounds for polycrystalline composites when the nonlinearity is subquadratic (joint work with J. R. Willis).

Bounds for Nonlinear Composites which Incorporate Morphological Information

Talbot, D.R.S.
Coventry University, United Kingdom

The nonlinear Hashin-Shtrikman variational structure relies on the introduction of a comparison material. In recent work a nonlinear comparison composite has been employed. This has enabled both upper and lower bounds to be found that depend on the three-point statistics of the microstructure through a parameter introduced by G. W. Milton. At least one of the bounds requires an estimate of the size of the trial field to be known and even if the best estimate available is used and the Milton parameter is known for a particular microstructure, the bounds can still be widely separated.

O. P. Bruno has obtained bounds for a linear composite consisting of a matrix containing spherical inclusions where the inclusions are coated with the matrix phase. The bounds remain nontrivial even when the properties of the inclusions tend to either zero or infinity. These bounds are used to improve the bounds for a nonlinear composite comprising either a nonlinear matrix containing linear inclusions or a linear matrix containing nonlinear inclusions. Results are presented in the context of dielectric composites.

Second-Order Estimates for the Effective Behavior of Nonlinear Polycrystals

Bornert, M.,
Laboratoire de Mécanique des Solides, France
and
Castañeda, P.P.
University of Pennsylvania, USA

A general theory for the prediction of the effective properties of nonlinear composites, which is exact to the second order in the contrast of the phases, has recently been proposed [1]. It is based on second-order Taylor expansions for the stress or strain potentials in each of the phases. Although this general theory applies to any type of heterogeneous material, it has up to now only been used for two-phase composite materials. The reason is that it relies on estimates for the effective properties of an anisotropic thermoelastic composite. These are easy to derive from estimates for anisotropic composites with identical phase distribution when there are only two phases: Levin's theorem can be applied in such a case.

For composites with more than two phases, such as polycrystals, the thermoelastic problem has to be dealt with explicitly. Following Willis [2], a variational formulation of the Hashin and Shtrikman type can be used to estimate the effective potential of the anisotropic thermoelastic composite. All the quantities involved in the procedure can be made explicit for the case of an isotropic distribution of the phases. When the anisotropic effective linear moduli of this composite are used as a reference material, self-consistent estimates are generated. The effective potential can then be derived from the general relations of the second-order theory. A double iterative scheme is necessary to numerically solve the nonlinear system of equations: the first is related to the self-consistent condition and the second to the determination of the average strain or stress in the nonlinear phases. Two different estimates can be generated, depending on which energy function is expanded: the stress or the strain energy.

The procedure is applied to a 2D model polycrystal for which a rigorous upper bound, improving on the classical Taylor bound for large grain anisotropy, has been proposed recently by Kohn and Little [3]. Unlike the classical self-consistent estimates (including Hill's incremental estimates), the proposed second-order estimates satisfy the Kohn-Little bound, as well as more restrictive bound due to Ponte Castañeda and Nebozhyn [4]. Applications to 3D polycrystals will also be discussed.

[1] P. Ponte Castañeda, 1996, *J. Mech. Phys. Solids* **44**, 8276-862.

[2] J. R. Willis, 1981, *Adv. Appl. Mech.* **21**, 1-78.

[3] R. V. Kohn and T. D. Little, 1997, *SIAM J. Appl. Math.*

[4] P. Ponte Castañeda and M. V. Nebozhyn, 1997, *Proc. R. Soc. Lond. A* **453**, 2715-2724.

Session: A3-4 Room: Cascade 127 **Time:** T3:30p-5:30p
Chairs: ***V. P. Smyshlyaev (University of Bath) & K. Bhattacharya (Caltech)***

Microscopic Misfit Strains in Polycrystals

Bruno, O.P.
California Institute of Technology, USA

I will present an approach to the solution of elasticity problems in two- and three-dimensional polycrystals supporting microscopic misfit strains. This approach is applicable to polycrystals whose grains or intergrain boundaries undergo arbitrary misfit deformations, such as those associated with thermal expansion, martensitic transformations, etc, possibly including grain boundary fracture. I will also present rigorous bounds for the calculated energy values, which result from relaxation of the statistics of the given polycrystal. Our numerics are based on consideration of a large number of exact Eshelby-type solutions in small discretization units together with a fast optimization algorithm (requiring a number of the order of *Nlog(N)* operations, where *N* is the number of discretization cells). Imposed boundary conditions interact with the misfits through the elasticity equations, and lead to a statistically correlated array of misfit strains. Explicit numerical results will be given for martensitic transformations in polycrystals. The accuracy of the numerical results, finally, will be demonstrated by comparison of the numerical energy values with our corresponding rigorous bounds.

Homogenization and Bounds for the Overall Elastic Energy of Martensitic Polycrystals

Smyshlyaev, V.P.
University of Bath, United Kingdom and
Willis, J.R.
Cambridge University, United Kingdom

For shape-memory polycrystals characterized by statistics (e.g. two-point correlation functions) of orientation distribution we propose a "Hashin-Shtrikman" type variational approach for estimation of the overall energy stored in the polycrystal subjected to an external mechanical loading. This in a sense develops and generalizes a recent approach of O.P. Bruno et al who employed the Eshelby solutions technique (this had an effect of allowing for non-constant strains and improved the Taylor upper bound). We discuss associated Hashin-Shtrikman type ``non-local" variational principle for the elastic energy of the polycrystal, which in a natural way builds a connection between the single crystal relaxation problem and the polycrystal energy minimization problem.

The variational principle is applied to derive upper bounds for a statistically uniform polycrystal. This has an effect of extending the approach of Bruno et al to more general orientation distribution statistics, and to polycrystals made of single crystals with "kinematically incompatible" transformation strains. The resulting upper bound appears also to be sharper than that of Bruno et al as a result of an improved optimization procedure.

We discuss finally a "non-convex duality" transformation behind the variational principle and relation to the non-linear version of the Hashin-Shtrikman approach of Talbot and Willis.

V.P. Smyshlyaev & J.R. Willis, "A non-local variational approach to the elastic energy minimization of martensitic polycrystals", Proc. R. Soc. Lond. A (1998) 454.

A Theory of Thin Films of Martensitic Materials with Applications to Microactuators, Part I

James, R.D.,
University of Minnesota, USA

We will describe a theory of shape-memory thin films which is motivated by the design of microactuators and micropumps. Shape-memory alloys are particularly attractive here: first, they have the largest work output per unit volume of any known actuator system and, second, fast heat transfer at small length-scales overcomes the frequency limitations of bulk materials.

In part I, we will describe a direct derivation of a theory of single crystal thin films, starting from three dimensional nonlinear elasticity augmented by a term for interfacial energy. The derivation involves no *a priori* choice of asymptotic expansion, and yields a frame-indifferent Cosserat membrane theory. In part II, we apply this theory to a multi-well energy appropriate for martensitic materials and describe how the martensitic microstructure in thin films can differ qualitatively from that of the bulk. We will also construct simple energy minimizing deformations --- tents and tunnels --- which could be the basis of simple microactuators and micropumps. Explicit results will be given for some material systems.

We will indicate how this theory can be extended to polycrystalline films and films subject to pressure loading. We also report on progress toward making martensitic thin films patterned according to these predictions. Finally, we will discuss briefly two recent developments: 1) the direct derivation of plate-shell-thin film theories including bending that requires no *a priori* assumption on the asymptotic form of the deformation, and 2) the direct derivation of continuum theory of deformable thin films beginning with quantum mechanics.

(Joint work with Kaushik Bhattracharya.)

K. Bhattacharya and R. D. James, "A theory of thin films of martensitic materials with applications to microactuators," J. Mech. Phys. Solids, in press.

A Theory of Thin Films of Martensitic Materials with Application to Microactuators, Parts II

Bhattacharya, K.
California Institute of Technology, USA

We will describe a theory of shape-memory thin films which is motivated by the design of microactuators and micropumps. Shape-memory alloys are particularly attractive here: first, they have the largest work output per unit volume of any known actuator system and, second, fast heat transfer at small length-scales over comes the frequency limitations of bulk materials.

In part I, we will describe a direct derivation of a theory of single crystal thin films, starting from three dimensional nonlinear elasticity augmented by a term for interfacial energy. The derivation involves no *a priori* choice of asymptotic expansion, and yields a frame-indifferent Cosserat membrane theory. In part II, we will apply this theory to a multi-well energy appropriate for martensitic materials and will describe how the martensitic microstructure in thin films can differ qualitatively from that of the bulk. We will also conduct simple energy minimizing deformations - tents and tunnels - which could be the basis of simple microactuators and micropumps. Explicit results will be given for some material systems.

We will indicate how this theory can be extended to polycrystalline films and films subject to pressure loading. We also report on progress toward making martensitic thin films patterned according to these predictions. Finally, we will discuss briefly two recent developments, 1) the direct derivation of plate-shell-thin film theories including bending that requires no *a priori* assumption on the asymptotic form of the deformation, and 2) the direct derivation of continuum theory of deformable thin films beginning with quantum mechanics.

(Joint work with Richard D. James.)

K. Bhattacharya and R. D. James, "A theory of thin films of martensitic materials with applications to microactuators," J. Mech. Phys. Solids, in press.

Continuum Models for Stick-Slip Interface Motion in Shape Memory Tensile Bars

Rosakis, P.,
Cornell University, USA and
Knowles, J.K.
California Institute of Technology, USA

In tensile tests performed on shape memory alloy specimens, stress-induced transformation sometimes occurs by the jerky movement of interfaces. The phase boundary moves in stick-slip fashion, alternating between motion and rest in rapid succession. The macroscopic load-extension relation is not smooth but exhibits teeth or serrations.

In recent continuum models of phase transitions, the kinetic relation governing the transformation is assumed to be monotonic, so that the driving force is an increasing function of phase boundary velocity. In addition, it is assumed to be homogeneous, or independent of the location of the interface.

We explore the implications of relinquishing the assumption of monotonicity of the kinetic relation. We consider both quasistatic and fully dynamic behavior of bars in tension. It is found that non-monotonic kinetic relations are responsible for a dynamic instability in interface propagation. This predicts stick-slip phase boundary motion and serrated macroscopic stress-strain curves at low loading rates, but smooth behavior at higher loading rates.

We also consider an alternative model where the kinetic relation is monotonic but inhomogeneous. This is intended to model the effect on interface motion of micro-ostacles or inhomogeneities. This model also predicts irregular interface motion and serrated stress-strain curves, in this case for all loading rates.

Session: A3-5 Room: Cascade 127 **Time:** W9:30a-11:30a
Chairs: *R. Weaver (U. Illinois) &*
R. W. Ogden (U.Glasgow)

On Non-Propagation of Acceleration Waves in Anisotropic-Elastic, Plastic Solids

Bigoni, D.
University of Bologna, Italy and
Loret, B.,
Institut de Mecanique de Grenoble, France

The influence of elastic anisotropy on elastic-plastic acceleration wave-speeds is analyzed when the elastic anisotropy is described by a second-order fabric tensor. For a particular-and physically sounding-structure of the elastic tensor, localization to a problem relative to elastic isotropy. Thus the analytic solutions available in the framework of isotropic elasticity can be used. Applications show the strong effects of elastic anisotropy on all the localization characteristics.

For non-associative flow-laws, flutter instability (corresponding to the occurrence of complex conjugate squares of wave-speeds) is considered. It is shown that, while this instability is precluded for elastic-plastic solids with elastic isotropy and obeying deviatoric associativity, this exclusion property is not preserved in the presence of anisotropic elasticity. Moreover, a perturbation in terms of an infinitesimal and "appropriate" anisotropy is shown to give rise to flutter.

Surface Wave Propagation in a Pre-Stressed Elastic Body with a Thin Elastic Surface Coating

Ogden, R.W.
University of Glasgow, United Kingdom and
Steigmann, D.J.
University of California-Berkeley, USA

In a recent paper [Proc. R. Soc. Lond. A453 (1997), 853-877] the authors have developed a nonlinear static plane strain theory of an elastic solid coated with a thin elastic film which incorporates both extensional and bending stiffness in its constitutive law. In subsequent papers the theory and its applications have been developed further with particular reference to the effect that the surface film has on the stability and bifurcation behaviour of the bulk solid. In this talk we describe the extension of the theory to include dynamic effects. In particular, we derive the equations governing the motion of the film (including rotatory inertia terms). The equations are then used to obtain the equations for an incremental motion superimposed on a static finite deformation. These are then applied to the prototype problem of surface wave propagation in a homogeneously pure strained half-space of incompressible elastic material with a surface film on its plane boundary. The secular equation for the wave speed is obtained in explicit form in respect of general constitutive laws for the film and bulk material, allowance being made for possible residual stress and moment in the film. For illustrative purposes, attention is then confined to a special class of constitutive laws for the bulk material, for which the secular equation becomes a quartic (contrasting with the cubic which arises for an uncoated half-space). Numerical results are then used to demonstrate the influence that the film and bulk material properties and the magnitude of the underlying finite strain have on the surface wave behaviour. Comparisons are made with the classical theory of surface waves in a half-space on which a thin surface layer is overlaid and with the theory of surface waves in a half-space coated with an elastic membrane supporting residual surface tension.

Wave Propagation in Piezocomposites

Sabina, F.J.
Universidad Nacional Autónoma de México, Mexico

A new theory has been developed for the analysis of the overall properties and the propagation of waves though inhomogeneous piezoelectric materials with randomly distributed microstructure. The self-consistent method has been used by means of a very simple instrumentation, which allows the prediction of resonance phenomena for wavelengths comparable to the diameter of the inclusions. This variant has already been shown to be very versatile and it has a good prediction capability since its wave characteristics compare well with experiments for the uncoupled counterpart problem in elasticity. Here the problem of predicting the overall properties for 0--3 connectivity piezocomposites and wave propagation through a piezoelectric matrix containing piezoelectric ellipsoidal inclusions, randomly positioned, but with a fixed orientation are studied. The single scatterer problem, which is needed as part of the implementation of the method, is posed as coupled integral equations for the polarizations of momentum density, stress and electric displacement using the piezoelectric Green's function for a transversely isotropic media. The integral equations are solved approximately by means of Galerkin's method. The implicit self-consistent equations are solved by iteration using a continuation method in the frequency for the overall elastic, piezoelectric and dielectric properties of the piezocomposite. From these an eigenvalue problem yields the phase speed and the attenuation of the waves

as a function of the frequency of the waves in a equivalent homogeneous, but attenuative, piezoelectric composite.

Radiative Transfer and Diffusion of Elastic Waves in Random Polycrystals

Weaver, R., University of Illinois, USA

Most study of elastic waves in random structures has emphasized the long-wavelength limit where ensemble or volumetric averages are relevant. At shorter wavelengths, however, an initially plane elastic wave loses its spatial coherence over distances comparable to, or shorter than, specimen length scales. A simple average is not sufficient for the characterization of such fields. An elastic wave that has undergone many randomizing scatterings generates a field that is termed "diffuse," or "grain noise." Such ultrasonic fields are increasingly being used for nondestructive evaluation.

A review is presented here of a perturbative, smoothing, theory for the evolution of mean square elastodynamic field due to a point force. It is shown that in certain limits (summarizable by the criterion al << 1, where a is attenuation and l is wavelength) the theory predicts that a radiative transfer equation (RTE) governs the field's specific intensity. In a further, late time, limit, it is found that the RTE reduces to a diffusion equation for the elastodynamic energy density.

More recently these procedures have been applied to the field generated, not by a point force, but by a model piezoelectric transducer. It has been found that the RTE needs suitable modification, and that specific intensity is not the right dependent variable. The appropriate modifications are discussed and the prospects for modeling the multiply scattered grain noise in polycrystals assessed.

Session: A3-6 Room: Cascade 127 **Time:** W1:00p-3:00p
Chairs: *S. Nemat-Nasser (UC-San Diego) & J.L. Bassani (U. Penn)*

Lattice Incompatibility and Nonlocal Crystal Plasticity

Bassani, J.L., University of Pennsylvania, USA

In continuum theory the crystal lattice is assumed to distort only elastically during plastic flow, while generally the elastic deformation itself is not compatible with a single-valued displacement field. Lattice incompatibility is characterized by a certain skew-symmetry property of the gradient of the elastic deformation gradient field, and this measure can play a natural role in a nonlocal theory of crystal plasticity. A simple constitutive proposal is discussed where incompatibility only enters the instantaneous hardening relations and the incremental boundary value problem has a classical structure. Preliminary predictions for size-scale effects in the torsion of thin wires and straining of thin films are promising.

A Theory of Single Crystal Plasticity with Microstructure

Ortiz, M., and Repetto, E.
California Institute of Technology, USA

Plastically deformed crystals are often observed to develop intricate dislocation patterns such as the labyrinth, mosaic, fence and carpet structures. In this paper, such dislocation structures are given an energetic interpretation with the aid of direct methods of the calculus of variations. We formulate the theory in terms of deformation fields and regard the dislocations as manifestations of the incompatibility of the plastic deformation gradient field. Within this framework, we show that the incremental displacements of inelastic solids follow as minimizers of a suitably defined pseudoelastic energy function. In crystals exhibiting latent hardening, the energy function is nonconvex and has wells corresponding to single-slip deformations. This favors microstructures consisting locally of single slip. Deformation microstructures constructed in accordance with this prescription are shown to be in correspondence with several commonly observed dislocation structures. Finally, we show that a characteristic length scale can be built into the theory by taking into account the self energy of the dislocations. The extended theory leads to scaling laws which appear to be in good qualitative and quantitative agreement with observation.

Finite Plastic Flow of Granular Materials

Nemat-Nasser, S.
University of California at San Diego, USA

Fundamentals of finite-deformation elastoplastic flow of densely packed granular materials which carry the applied loads through contact friction, are discussed, integrating the material behavior at three distinct length scales, i.e., the micro-scale, the meso-scale, and the macro-scale. Considering the contact forces, contact normals, and branches (which are vectors connecting the centroids of two adjacent contacting granules), at the micro-scale, expressions for the overall stress tensor, and the tractions transmitted across interior macroscopic planes, are developed. Macroscopic parameters which characterize the microstructure and its evolution in the course of deformation, are identified in terms of fabric tensors and the distribution density functions of unit branch vectors and contact normals, leading to explicit relations between the stress and fabric tensors. At the meso-scale, the deformation is assumed to consist of dilatant simple shearing over several interacting sliding planes. Resistance to such simple shearing is provided by friction due to rolling and sliding at the micro-scale, and restructuring through redistribution of the contact

normals, i.e., the change in the fabric. An explicit expression is obtained for the critical value of the resistive shear stress, by integrating the corresponding contact forces over a typical sliding plane. Finally, physically-based continuum constitutive relations are obtained, based on the double sliding-plane model which includes dilatancy (densification), pressure sensitivity, and, most importantly, the anisotropy due to the fabric structure which enters into the resulting continuum constitutive relations through a back stress.

Nemat-Nasser, S., "On Behavior of Granular Materials in Simple Shear," *Soils and Foundations*, Vol. 20 (1980), 59-73.

Christoffersen, J., M.M. Mehrabadi, and S. Nemat-Nasser, "A Micromechanical Description of Granular Material Behavior," *Journal of Applied Mechanics*, Vol. 48 (1981), 339-334.

Oda, M., S. Nemat-Nasser and M.M. Mehrabadi, "A Statistical Study of Fabric in a Random Assembly of Spherical Granules," *International Journal for Numerical and Analytical Methods in Geomechanics*, Vol. 6 (1982), 77-94.

Balendran, B. and S. Nemat-Nasser, "Double Sliding Model for Cyclic Deformation of Granular Materials, Including Dilatancy Effects," Journal of Mechanics and Physics of Solids, Vol. 41, No. 3 (1993), 573-612.

A Generalized Peierls-Nabarro Model of a Dislocation in a Discrete Lattice

Movchan, A.B.
University of Bath, United Kingdom
Willis, J.R.
University of Cambridge, United Kingdom and
Bullough, R., United Kingdom

The classical linear continuum approach of Hirth and Lothe for modelling an edge dislocation in a crystal yields singularities of stress and strain at the dislocation line. An alternative semi-continuum model was constructed by Peierls and Nabarro, who assumed a nonlinear discrete sinusoidal interaction between the layers of atoms on each side of the glide plane. In the latter case the strain components are bounded.

A dislocation exists in a discrete atomic lattice, and therefore, a physical model of such a dislocation should have some correspondence to a discrete lattice. As the external shear stress reaches a certain critical value (the so-called Peierls stress), the dislocation moves through the lattice. The algorithm for evaluation of the Peierls stress, developed by Nabarro, involves a combination of a discrete representation for the misfit energy and a solution of a homogeneous singular integral equation (continuum model).

To obtain the Peierls stress it would be natural to introduce a non-zero constant term (corresponding to an external shear stress), to solve the nonhomogeneous Peierls equation for increasing external shear stress and to identify the critical external shear stress for motion of the dislocation. However, the Peierls solution does not allow for small perturbations corresponding to an additional infinitesimal constant term in the equation. This situation explains the reason for Nabarro's choice to use the lattice model for evaluation of the misfit energy and to employ the solution of the homogeneous Peierls equation, to provide the corresponding "atomic" configuration.

We develop a discrete analogue of the Peierls-Nabarro model which describes simply and accurately the nonlinear interaction of two harmonic lattice half-spaces. The evaluation of the critical stress required to move the dislocation through the lattice and the dependence of the critical stress on the dislocation width are studied systematically on the basis of stability analysis of solutions of a certain evolution problem; this approach is different from that employed by Nabarro, and it is mathematically rigorous. This approach is extended to the analysis of model of a dipole and to the study of dislocation kinks in three dimensions.

Session: A3-7 Room: Cascade 127 **Time:** W3:30p-5:30p
Chairs: *A.J. Rosakis (CalTech) &*
N. V. Movchan (U. Bath)

Nonlinear Fracture Mechanics of Piezoelectric Ceramics

Fulton, C.C. and Gao, H.
Stanford University, USA

The design of smart structures using piezoelectric transducers depends on an accurate assessment of the potential failure modes of these materials. Unfortunately, the linear fracture mechanics theory cannot be reconciled with observed cracking behavior under combined electrical and mechanical loading conditions. The discrepancies between theoretical predictions and experimental findings indicate that nonlinear material effects may play a significant role. With the goal of developing a more realistic fracture criterion for piezoelectric ceramics, we examine the crack tip at a length scale dominated by electrical nonlinearity, assuming that plastic yielding remains negligible. At this level of magnification, material inhomogeneities such as individual grains or polar domains can be considered as discrete electric dipoles superimposed on a medium with globally averaged material properties. Because of the steep gradients in the electric field, the crack exerts a net force on nearby dipoles. As a result, the local energy release rate differs from the crack driving force observed from a macroscopic perspective, at which the effects of varying polar domains are homogenized. In some cases, the local energy release rate is independent of the positions and strengths of the dipoles and an analytical expression can be obtained. The model shows promise for explaining the failures of cracked specimens under electromechanical loads.

Mathematical Modelling of Fracture in Fibre-Reinforced Ceramic Materials

Movchan, N.V.
University of Bath, United Kingdom and
Willis, J.R.
University of Cambridge, United Kingdom

A typical failure process in fibre--reinforced ceramics is characterized by formation of a matrix crack which extends through the composite leaving unbroken fibres behind its front. The intact fibres debond from the matrix and then act as bridging ligaments in the crack wake reducing the intensity of the stresses near the crack tip. One convenient method to analyze this phenomenon is to ``smear out'' the fibres and account for their influence by admitting a continuous distribution of cohesive traction γ across the crack faces, with the traction specified as a function of the local crack--face separation φ The problem is then formulated in terms of a hypersingular integral equation for the relative crack-face separation φ The distribution of restraining traction, provided by fibres, is described by a nonlinear force-separation law $\gamma(\varphi)$ the form of which will depend upon the mechanics assumed for the fibres embedded in the matrix.

When fibres are lying perpendicular to the crack plane, as in aligned fibre composite loaded in the fibre direction, crack bridging stress arises from the stretching of debonded fibres. For such a case, the representation for $\gamma(\varphi)$ can be derived by considering a more refined model of the crack bridging which accounts for interaction between fibres and for frictional sliding at the fibre-matrix interface. The basic idea of the method is to express the stress and displacement fields in the composite in terms of the solution of a model problem for a single fibre in an ambient stress field produced by all other fibres and applied load. The study is restricted to fibres held in place by Coulomb friction.

The objective is to analyze in three dimensions the effect of a random array of discrete fibres bridging a crack, to assess the error incurred in using the "continuous bridging" approximation. Near the tip of the crack, the stress fields display strong spatial variation. The fibres interact not only with each other but also with the crack tip, and the latter interaction invalidates the use of the unique $\gamma(\varphi)$ relation, which applies when the (locally averaged) stresses vary slowly with the position on the crack surfaces. We consider two problems: a semi-infinite bridged crack in a uniform stress field, and a crack in a stress field generated by a pair of unit body forces. We present the results that indicate the dependence of the solution of the problem on material parameters, the value of applied load and the distance from the crack front.

Dynamic Shear-Dominated, Intersonic Crack Growth in Bimaterial and Layered Systems

Rosakis, A.J.
California Institute of Technology, USA

Dynamic cracks propagating in the interfaces between materials characterized by a high mismatch in wave speeds (e.g. metal/polymer) are studied using optical techniques and high-speed photography. These cracks accelerate, within microseconds, to the shear wave speed, (C^1_S ~ 1000 m/s), of the more compliant of the two solids (solid -1). At this speed they propagate in a stable manner until enough excess energy is supplied to the system. Subsequently, they further accelerate to supersonic speeds, ($v>C^1_L$ ~ 2000 m/s), with respect to the polymer side, eventually reaching the Rayleigh wave speed of the metal, C^1_L ~ 3100 m/s. Such cracks become almost completely shear dominated and exhibit large scale contact between the crack faces. They also feature the distinct shock wave structure expected of intersonically or supersonically moving disturbances. Intersonic crack growth along the fibers of unidirectional graphite/epoxy composite plates is also presented. Here also, shock waves are visible and the crack speed is as high as 6,000 m/s. This is the first time that intersonic and supersonic crack growth has ever been reported in a laboratory setting. However, in a much larger scale, such processes are known by geologists to occur in stratified layers within the earth's crust. These recent laboratory observations have stimulated theoretical and numerical interest in dynamic shear rupture. A number of such models are discussed vis a vis their ability in predicting the experimental observations.

On The Analysis of Dynamic Unsteady Crack Growth in Elastic Material

Walton, J.R., and Leise, T.
Texas A&M University, USA

In this symposium honoring John Willis, it seems fitting to report on some recent progress in constructing solutions to dynamic fracture problems, one of the many areas of applied mechanics to which Professor Willis has made seminal contributions. The problems of interest in this talk concern the unsteady, dynamic growth of planar cracks in elastic material. Most existing closed form solutions to such problems have been for a single semi-infinite crack propagating in an infinite isotropic, homogeneous linear elastic or viscoelastic material. The authors report here on a method by which closed form solutions can be constructed for multiple, finite length, dynamically accelerating, co-planar cracks. In particular, expressions are constructed for crack opening displacements as well as stress intensity factors for such problems. The specific results presented here are

in the context of anti-plane shear deformations in linear elastic material, but in principle the method can be applied to plane strain deformations and to viscoelastic as well as elastic material. One of the applications of these solutions is to the study of the process by which multiple, co-planar micro-cracks grow and coalesce into a macro-crack which is an important mechanism for damage development in many brittle materials.

Symposium B1
Numerical Modeling of Flow around Bluff Bodies
Organizers
S. Parameswaran, Texas Tech University, USA
A. Hadid, Boeing, USA
V. Sumantran, General Motors, USA
R. Sun, Chrysler, USA, &
S.S. Ravindran, NASA, USA

Session: B1-1, Room: CUB B7-9, **Time:** M10:00a-12:00p
Chairs: *A. Hadid (Boeing) &*
S. Parameswaran (Texas Tech)

Turbulence Modeling, Validation and Technology Transfer

Huang, P.G.
University of Kentucky, USA

CFD (Computational Fluid Dynamics) has become a critical tool in the aerospace industry in both application and research and development. One of the critical components in successful CFD predictions is a correct choice of turbulence models. Unfortunately, due primarily to the inefficient and crude method of transfer of modern turbulence models to the CFD community, CFD has not kept pace with the progress made with turbulence models. As a result, the choice of the models is generally not obvious to CFD code developers or application engineers.

A project is described to transfer turbulence model technology for CFD to industrial and government institutions by ways of a "living" expert system, essentially an intelligent database and Code Validation System, which contains experimental data, model descriptions, solution algorithms and detailed model comparisons. This system can provide information archiving and sharing capabilities for large groups collaborating on specific CFD projects. The data base will be used by the CFD code developers to validate their coding for a specific turbulence model and by CFD design engineers to select an appropriate model for their specific CFD design applications. One goal is to keep the CFD community "up to speed" on progress made in turbulence modeling.

The timely transfer of this critical knowledge would help ensure that U.S. industry and government research scientists keep pace with current trends and progress made by turbulence modelers.

Les Simulation of Turbulent Obstacle Flow Using Eddy-Viscosity Type Subgrid Models

Hadid, A.H., and Sindir, M.M.
CFD Advanced Analysis, USA and
Parameswaran, S.
Texas Tech. University, USA

Accurate simulation of flows around bluff bodies is of paramount importance in many industries such as aerospace and automotive among others. The structural integrity and performance of many products are affected by the dynamic loads of unsteady flow fields they encounter. Accurate and efficient calculations of vortex shedding phenomenon are quite sensitive to the turbulence models used and to the numerical algorithm.

The work described in the present paper attempts to analyze the detailed flow characteristics behind a square cylinder mounted on one wall. Flow simulations using two eddy-viscosity type subgrid models are presented; one is based on the Smagorinsky model with Van-Driest damping near the walls, while the second one is based on the algebraic RNG model of Yakhot and Orszag with no damping. The numerical platform is based on a high order Legendre spectral element spatial discretization with second order temporal accuracy. Systematic evaluation of the numerical method and physical models will be included together with detailed characteristics of the salient features of the flow and comparisons with available data.

Complex Vortex Dynamics in Bluff-Body Wakes

Mittal, R.
University of Florida, USA

As computing power has increased in recent years, direct-numerical simulation (DNS) of bluff-body wakes at low Reynolds numbers (Re_D<1000) has become feasible and this has played a major role in advancing our knowledge of these flows. The circular cylinder can be considered a prototypical 2-D bluff body whereas its counterpart in 3-D is the sphere. In our group, both these flow have been studied in detail with the aid of spectral-method based DNS solvers. The variety and complexity of the vortex dynamics that is exhibited in these wakes even at low Reynolds numbers is quite staggering and is the main focus of the current study. As the Reynolds number is increased, the sphere wake undergoes a sequence of bifurcations, which is significantly different from what is observed in the cylinder wake and the current study will elucidate the similarities and differences between these flows. Detailed comparisons of the formation and evolution of vortical structures in the wake will be made with particular emphasis on describing some peculiarities of the sphere wake. The response of these wakes to freestream perturbations is of direct relevance to fluid-structure interaction and particulate flows and

results of our recent investigations into this issue will also be presented.

Influence of Turbulence Models on the Prediction of Vortex Shedding from a Bluff Body

Issa, R.I.
Imperial College of Science, London

One of the most challenging phenomena to turbulence models is vortex shedding from bluff bodies. It is now well established that numerical simulation of the phenomenon is quite sensitive to the models introduced to represent turbulence. In particular, the most popular of these models, k-ε, fails spectacularly to reproduce the strength of the vortices shed. This serious deficiency was traced back by Launder and Kato to the artificially high generation of turbulence energy at the forward facing stagnation point where in reality very little turbulence exists. The incorrectly predicted high level of turbulence leads to large effective viscosities which tend to suppress the extent of separation, thereby resulting in incorrect magnitudes of the oscillations in the flow field. The proposal by Launder and Kato for splitting the generation term in the k-ε equation into two terms relating to strain and vorticity, produced the desired effect; however, the approach was not sufficiently rigorous to be widely accepted.

The work described by the present paper relates to the computation of vortex shedding from a square cylinder using a finite-volume numerical method. Both the standard k-ε model and its RNG variant are used and the flow is modelled as a two-dimensional problem. The results of the computations are compared with the data of Durao, Heitor and Pereira. It is first explained that the results of the simulations are extremely sensitive to the values of turbulence quantities specified at inlet as well as to the location of the inlet itself relative to the body. It is normal practice to limit the domain of computation upstream of the cylinder to only a few cylinder heights; this is done in order to make the computational resource need manageable. However, it is found that such a practice can considerably affect the outcome of the calculation and yield significantly weaker vortices than in reality. It is reasoned that perturbations in the flow field (especially in pressure) propagate far upstream and possibly beyond the point where the inlet boundary is placed. The steady state boundary conditions imposed at inlet therefore tend to suppress these perturbations and force the flow to be nearly steady upstream of the obstacle. The net result is an attenuation of the ensuing oscillatory motion of the flow around the body. The computations presented are all made with the full geometry of the experimental flow configuration extending all the way to the actual inlet of the wind tunnel.

The computed results show that even with the appropriate extension of the calculation domain, the standard k-ε model under predicts the strength of the vortices shed. On the other hand, the RNG variant of the model does much better in predicting the magnitudes of the fluctuations in velocity. It is shown that this model predicts much less turbulence at the front stagnation point due to the stronger dissipation effect characteristic of the model. If one follows the argument of Launder and Kato, then it becomes clear why the model is able to predict the vortex shedding process reasonably correctly.

The paper will also compares the turbulence model results with independent LES calculations performed for the same case. It is shown that LES results are indeed superior to the turbulence model ones as expected. However, the degree of improvement is perhaps not so drastic in this case due primarily to the fact that the RNG variant of the k-ε model produces fairly satisfactory results in the first instance.

On Large Eddy Simulation of Flow Over a Cylinder

Moin, P.
Stanford University, USA

Session: B1-2 Room: CUB B7-9 **Time:** M1:30p-3:30p
Chair: *V. Sumantran (GM)*

Flow Induced Noise from Ground Vehicles - Problems and Prospects of Numerical Simulation

Ahmed, S.R.
DRL, Institute of Design Aerodynamics, Germany

The continuing increase in automobile and utility vehicle population in industrialised and developing countries has led to these vehicles being identified as the prime source of noise in urban areas and on the highways. Polls conducted over the years in Germany show that over 70% of the population currently feel subjected to serious annoyance through traffic noise. This result may also be true for other industrialised countries.

Demands on comfort and prevention of noise induced fatigue during long driving periods is becoming an important car purchaser requirement. For the continued acceptance of automobiles in the future, car and utility vehicle manufacturers have to solve the technical problems involved in designing vehicles which are quieter both inside and outside.

Even though the degree of discomfort through noise may be subjective, measurable quantities defining noise and means to reduce them are the

engineering approach to reduce the annoyance impact of noise.

This paper attempts to review the current technology available to predict the noise generated by the various sources on ground vehicles during their motion. The emphasis would be on flow induced noise and analysis of the noise generating mechanisms.

From aerodynamic viewpoint, a ground vehicle is a bluff body moving in ground vicinity. The noise generated is the consequence of the complex flow field generated during its motion. A prediction of the overall flow with a detailed and correct physical description of the salient flow features is a prerequisite for an aeroacoustic computation and analysis. Problems and prospects for the CFD simulation of bluff body flows will be addressed.

An Analysis of Some Numerical Simulation Issues Related to Bluff Body Aeroacoustics

Chakravarthy, S.R., Palaniswamy S., Peroomian, O., and Goldberg, U.C.
Metacomp Technologies, Inc., USA

The difference in the order of magnitude of pressure fluctuations associated with fluid dynamics and acoustics necessitates separation of the scales. The case for decoupled fluid dynamics and acoustics and the case for coupled but separate fluid dynamics and acoustics is explored from a numerical viewpoint. The types of aeroacoustic phenomena that are adequately resolved by numerical simulation of the Reynolds-averaged Navier-Stokes equations and those that require the use of special acoustics equations (e.g. linear wave equation formulations) is delineated. We attempt to study the following aspects:

When solving the Euler or Navier-Stokes equations, under what conditions are engineering methods (second order spatial and temporal accuracy) sufficient and when is it necessary to use higher-order (e.g. 4^{th} order) methods. The availability, applicability and efficiency of such higher order methods for complex geometries and topologies.

When solving the acoustics equations, the need for higher order accuracy and the need for reduced numerical dissipation. The various approaches available to achieve higher order schemes for linear equations.

A brief comparative survey of methods that are designed in Taylor-series space and analyzed in Fourier space vs. those designed in Fourier-space and whose properties are analyzed in Taylor-series space.

Coupling of the numerical solution of the Navier-Stokes equations with the numerical solution of the acoustics equations.

The adequacy of dual time-stepping methods to perform time-dependent aeroacoustics of bluff bodies.

Numerical dissipation and accuracy effects in representing vortex phenomena accurately and the resulting impact on unsteady effects.

The role of far field boundary conditions.

The role and adequacy of turbulence models in the prediction of bluff body aeroacoustics.

Computation of Trailing Edge Noise Using Large Eddy Simulation

Moin, P, and Wang, M.
Stanford University, USA

Turbulent boundary layers near the trailing-edge of a lifting surface are known to generate intense, broadband scattering noise as well as surface pressure fluctuations. To numerically predict the trailing-edge noise requires that the noise-generating eddies over a wide range of length scales be adequately represented. This requirement cannot be met by the traditional CFD methods based on Reynolds-averaged Navier-Stokes (RANS) equations or Euler equations.

The objective of this work is to develop numerical prediction methods for trailing-edge aeroacoustics using a combination of large-eddy simulation (LES) techniques and aeroacoustic theory based on Lighthill's analogy. With this approach, the turbulent flow field near the trailing-edge is obtained by means of LES. The space-time evolution of the surface pressure fluctuations, useful as forcing function for structural vibration models, is also computed directly. The simulation results allow the acoustic source functions, or the fluctuating Reynolds stress, to be evaluated. The radiated noise can then be computed from an integral-form solution to the Lighthill equation using a hard-wall Green's function (Ffowcs Williams & Hall, *J. Fluid Mech.*, Vol. 40, pp. 657-670, 1970).

Simulations have been carried out for a flow past a flat strut with an asymmetrically beveled trailing edge, of the type investigated experimentally by Blake (DTNSRDC Report 4241, David Taylor Naval Ship R & D Center, Bethesda, Maryland, 1975), at a chord Reynolds number of 2.15×10^6. The asymmetric edge shape produces a separated boundary layer on one side and an attached boundary layer on the other. The LES is based on the unsteady, incompressible Navier-Stokes equations, and employs the dynamic subgrid-scale model. The computational domain contains the aft section of the strut and the near-wake. The mean and turbulent velocities at the inflow boundary are provided through an auxiliary RANS calculation in a larger domain enclosing the entire strut, and a flat-plate boundary layer LES, respectively. Several simulations have been conducted to assess the effects of grid resolution and inflow velocity profiles. The computational results, including velocity and unsteady surface pressure statistics, compare reasonably well with Blake's experimental measurements.

Computational Aeroacoustic Analysis System Development

Hadid, A.H., Lin, W., Ascoli, E., Darian, A., Stewart, M., Barson S., and Sindir, M.
Boeing North American Inc., USA

Many industrial and commercial products operate in a dynamic flow environment and the aerodynamically generated noise has become a very important factor in the design of these products. In light of the importance in characterizing this dynamic environment, Rocketdyne has initiated a multiyear effort to develop a general-purpose computational aeroacoustic analysis system. This system will provide a high fidelity predictive capability for aeroacoustic design and analysis. The numerical platform is able to provide high temporal and spatial accuracy that is required for aeroacoustic calculations through the development of a high order spectral element numerical algorithm. The analysis system incorporates a graphical user interface (GUI) through PATRAN to provide access to all the necessary tools. These include preprocessing (geometry import and grid generation and boundary condition specification), code set up (problem specification, user parameter definition, etc.), and postprocessing.

The purpose of the present paper is to assess the feasibility of such a system and to demonstrate the efficiency and accuracy of the numerical algorithm through a numerical example. Computations of vortex shedding noise were carried out in the context of a two-dimensional low Mach number laminar flow past a cylindrical body. The computational aeroacoustic approach utilized in the present study consists of two parts. First, the time dependent incompressible flowfield is calculated using a high order numerical algorithm and then the acoustic field is calculated using linearized Euler equations. The unsteady fluid motion which is responsible for both the generation and propagation of acoustic waves is calculated using a high order spectral element method that accurately model complex geometry and rapidly varying flow field. The acoustic field is governed by the linearized Euler equations derived from the perturbation expansion about Mach number.

Model Equations for the Calculation of Deforming Surfaces in Non-Steady Flows

Warsi, Z.U.A.
Mississippi State University, USA

The purpose of this paper is to develop certain model equations for the prediction of deforming and moving surfaces in non-steady flows. A pertinent problem in this regard is the prediction of changing shock surfaces in front of a body in non-steady motion. The key idea here is to develop a non-steady coordinate generator which is to be used in the generating equations were developed earlier by the present author, Warsi [1]. In this paper, we will follow the notation and convention used in references [1] and [2]. To introduce the idea of non-steady coordinates, we refer to [2] and we consider a surface which is deforming in time. Denoting the surface coordinates which are time dependent as x^{δ}, δ = 1,2, the surface grid equation is considered in the form

Equation (1) is the fundamental equation for the generation of non-steady coordinates in a deformable surface. In the ensuing calculation, we have taken $\phi=1\langle G_3$. Suppose we wish to generate coordinates in a

$$\phi \frac{\partial r}{\partial \tau} = \frac{1}{G_3}\left(- r - G_3(k_I + k_{II})n - \phi G_3 \frac{\partial r}{\partial x^3}\frac{\partial x^3}{\partial t}\right) \quad (1)$$

moving and deforming shock surface and further we use a spectral methodology to solve Eq. (1). Referring to Ref. [3] we take $x^3=n$, the distance normal to the surface. It is straightforward to show that

$$\frac{\partial \mathrm{r}}{\partial \mathrm{n}} = \mathrm{n}, \frac{\partial \mathrm{n}}{\partial \mathrm{t}} = -\mathrm{r}_{\tau} \bullet \mathrm{n} = -\mathrm{q}_{\mathrm{s}}$$

The important point to note here is that the shock speed q_s must come from the calculation of the flow field. In order to demonstrate the applicability of Eq. (1), we have specified q_s arbitrarily as

$$q_s = \left(1 - \left|\cos(\alpha\tau)\right|\right) G_3(k_1 + k_u)$$

Solution of Eq. (2) shows significant deformation of the shock surfaces under the hypothetical function q_s.

[1]Z.U.A. Warsi, *J. Comput. Phys.*, 64, 82, (1986).
[2]Z.U.A. Warsi, *Fluid Dynamics: Theoretical and Computational Approaches*, CRC Press Inc., (1993).
[3]Z.U.A. Warsi, *AIAA Journal*, 35, 1228, (1997).

Session: B1-3 Room: CUB B7-9 **Time:** M4:00p-6:00p
Chair: *S. S. Ravindran (NASA)*

Advances in Optimal Control of Navier-Stokes Equation

Sritharan, S.S.
Space & Naval Warfare Systems Center, USA

During the past ten years several fundamental advances have been made in the control theory of viscous time dependent fluid dynamics covering deterministic, stochastic and H-infinity methods. In this talk we will give a flavor of the developments as well as some future directions. Some of the mathematical structures involved include Hamilton-Jacobi theory in infinite dimensions and also martingale problems in infinite dimensions.

Adaptive Shape Sensitivity Calculations in Thermal Fluids

Borggarrd, J.
Cornell University, USA

Optimal design problems frequently take the form of minimizing an objective function that depends on the design parameters through the solution of a partial differential equation. An expression for the gradient of this objective contains terms that are governed by the so-called sensitivity equation. In this talk we focus on an application where these PDEs are given by the Navier-Stokes equations (to model a thermal fluid) and the design parameters describe the shape of the domain. A natural approach to find approximations to these optimal design problems is to cascade a numerical solution of the PDEs with an optimization algorithm. We consider a technique for finding approximations to both the objective function and its gradient using the same adaptive finite element technique. This approach raises convergence issues since the operations of differentiation and approximation do not commute. Thus the computed gradient is not consistent with the objective function computations. These issues are addressed in this talk and numerical results are provided.

Active Flow Control

Chokani, N.
North Carolina State University, USA

Flow separation occurs in a diverse range of flow conditions and geometry. This phenomenon is responsible for aerodynamic noise radiation, poor pressure recovery, pressure drag increase and wall pressure fluctuations. Consequently a substantial body of research, analytical, experimental and computational has been directed towards developing techniques to control the adverse effects of flow separation. In the present talk we assess the reliability of time-accurate Reynolds-averaged based Navier-Stokes simulations to study the salient features and to provide insight into the flow physics. The flows examined include: the unsteady flow over a cavity; the unsteady separation over a ramp; and the separation over an airfoil. The use of active flow control techniques using jet blowing and vortex generator jets to suppress the adverse effects of flow separation are demonstrated. It is also shown that the results of the simulations provide details of the mechanisms of the flow control.

Optimal And Robust Reduced—Order Feedback Control of Turbulent Channel Flows

Cortelezzi, L., Speyer, J.L., Lee, K-H. and Kim, J., University of California, USA

Optimal and robust reduced-order feedback control of near-wall turbulence in a channel flow is investigated. Controllers able to analyze distributed measurements and coordinate distributed actuators are considered. Blowing and suction at the wall of the channel are the means for suppressing near-wall disturbances. Measurements of wall-shear stresses to be fed back to the controller are provided by sensors distributed along the wall of the channel. Linear quadratic Gaussian (LQG) design, or, in modern terms, *cal* H_2 design, in conjunction with model reduction techniques is used to derive optimal and robust feedback controllers. The cost of the wall-shear stresses being non-zero and the cost of implementing the controller itself are accounted for by introducing an optimal performance index, or cost function. Optimal controllers robust with respect to disturbances of the process and measurements as well as to system parameter uncertainties are derived. Control design is shown to decouple with respect to wave numbers. Parallel design and parallel computation of the control algorithms are discussed. Implementation of the controllers in practical engineering applications is elaborated. Controllers' performances are tested on direct numerical simulations of turbulent channel flow. Substantial modification of the structure of near-wall turbulence and significant drag reduction are obtained.

Session: B1-4 **Room:** CUB B7-9 **Time:** T3:30p-5:30p
Chair: *R. Sun (Chrysler)*

Advances Towards Automated Aerodynamic Simulation Using Adaptive Cartesian Grids and Parallel Computers

Przekwas, A.J. and Wang, Z.J.
CFD Research Corporation, USA

The talk will present recent developments towards automated aerodynamic simulation. Automation is emphasized because the ultimate users of CFD tools are designers, who are not necessarily CFD experts. There are, however, different possible routes by which one can achieve automation. The most promising one seems to be the use of unstructured and adaptive grid based methodology. One particularly attractive griding approach - "viscous" adaptive Cartesian grid - will be discussed in detail.

The talk will cover the following issues:

- Geometric modeling, NURB-surface based and solid-based geometric modeling techniques will be discussed;
- Adaptive Cartesian/adaptive prism/projection grid generation method for complex geometries will be presented. Pros and cons of both methods will be illustrated;
- Implementation on parallel architectures based on the paradigm of domain decomposition and messaging;
- Solution-based grid adaptation, which is critical in achieving automated aerodynamic simulation. Several adaptation criteria will be demonstrated;

- Demonstrated cases will include both automotive and aerospace aerodynamic applications.

Computational Analysis for Bluff Body Aerodynamics

Han, T., General Motors Research and Development Center, USA

Reducing the drag on bluff bodies in ground proximity has important practical applications to ground vehicles. In contrast to the situation in aeronautics, where flow separation from body surfaces is largely avoided, ground vehicles inherently exhibit significant regions of flow separation. It is often observed that the drag coefficient is not sensitive to the forebody shape if the flow over the forebody is free from large-scale separations. However, flow separation on the afterbody of ground vehicles is unavoidable and this separation is the major source of aerodynamic drag for ground vehicles. Reducing the aerodynamic drag produced by the afterbody becomes one of the most important subject in bluff body aerodynamics. Computational Fluid Dynamics (CFD), as one of the CAE tools, has enjoyed growing popularity for analysis of many airflow situations, including ground vehicle aerodynamics. Three-dimensional Navier-Stokes analysis was applied to optimize the rear-end shape of a vehicle-like body in ground proximity. The flow analysis was coupled with an optimization program to find values of the shape parameters that produce a minimum aerodynamic drag. The approach of this method is to create a localized quadratic approximation to the objective function, in this case drag coefficient, in terms of the shape parameters. Values of the objective function is updated and used to select a new geometry, and the iteration process is repeated until the objective function converges to a minimum drag.

Wind Tunnel Design Optimization Utilizing Analytical Fluids

Gleason, M.
Chrysler Technical Center, USA

One of the last bastions of the design of engineering devices that uses a purely experimental approach is the design of the wind tunnels. A rather significant body of information developed during the early NACA days has served to aid in the design of a multitude of wind tunnels. However, this limited the solutions to the realm of design parameters that had already been examined and limited the degree of innovation. But with the advent of more powerful and accurate analytical approaches to fluids design, the ability to more closely examine the relevant fluid phenomena and design elements becomes available to the wind tunnel designer. The activity illuminated here deals with the design of a semi-open jet wind tunnel for the aerodynamic and acoustic development of automobiles. During the early design phases, many options were examined to enhance the performance and reduce the cost of the new full-scale facility that is to be built at the Chrysler Technical Center. Some of the many areas examined and improved were the corner and turning vane designs, the contraction (nozzle), a wide-angle diffuser, and the test section plenum, nozzle and collector. Both traditional Computational Fluid Dynamics (CFD) tools and the more recently developed digital physics approaches to analysis were utilized where their strengths were best exercised. The identification of the generation of coherent vortex structures around the semi-open jet airstream was identified and several approaches to minimizing their formation were examined. Experimental verification of these solutions was conducted to validate the final design adopted.

Using CFD as a Tool in Wind Noise Prediction

Strumolo, G.S.
Ford Motor Company, USA

Wind noise is a major problem in automobiles today. It is especially significant since powertrain and tire noise continue to diminish and quieter electric vehicles are on the horizon. Currently, wind noise is measured by placing the vehicle in a wind tunnel and monitoring the driver's ear position with either a microphone or head device. This is a costly procedure in both time and money that requires an actual vehicle to test and an acoustic-quality wind tunnel. Since we would like to examine the effect of exterior design changes on interior noise levels early in the program, auto companies would like the ability to start with a CAD model of the vehicle and compute the wind noise without any physical testing. This is a major problem, as it involves the accurate prediction of the exterior aerodynamic flow and the mechanism of noise transmission through the glass surfaces.

Computational Fluid Dynamics (CFD) can be used to help solve this problem. One way is to use the steady-state exterior flow solution, empirical pressure spectra taken from experiments, and a Statistical Energy Analysis approach to predict the interior noise. This is the basis of the *Wind Noise Modeller* tool developed at Ford. The theory behind this model will be described and applied to the Ford Taurus. The more ambitious approach would be to directly compute the time history of surface pressures all along the glass surfaces. From this we could compute the pressure spectra directly for the specific vehicle design. Progress towards this approach will also be discussed. The CFD tool used in both methods uses the Lattice Gas Method, commercialized by the Exa Corporation. A brief description of the approach behind this method will also be given.

Gary S. Strumolo is a Senior Staff Technical Specialist at the Scientific Research Laboratory of

Ford Motor Company. For the past five years he has been involved in developing techniques for coupling computational aerodynamics and aeroacoustics. Much of his recent work centered around methodologies for predicting interior sound due to wind noise.

Symposium B2
Dynamics of Particles in Fluids in Dense Two-Phase Flows
Organizer
C. T. Crowe
Washington State University, USA

Session: B2-1 Room: CUB B7-9 **Time:** T9:30a-11:30a
Chair: *C. T. Crowe (WSU)*

Discrete Particle Simulation of Granular Materials and Multiphase Flows

Tsuji, Y., Tanaka, T. and Kawaguchi, T.
Osaka University, Japan

The present authors who have been engaged in numerical analysis of granular materials and multiphase flows are particularly interested in cases where particle-to-particle interaction has significant effects on the phenomena. To treat this interaction mathematically, techniques named DEM or DSMC have been developed. Concerning the particle-to-particle interaction, two cases are considered: the one is collision-dominated flows and the other is the contact-dominated flows. DEM is for the contact-dominated flows and DSMC method is for the collision-dominated flows. DEM has been developed in the field of soil mechanics while DSMC is a technique developed in rarefied gas. Combining DEM and DSMC with CFD (computer fluid dynamics), the discrete particle simulation becomes more practical because not only the particle-particle interaction but particle-fluid interaction can be handled. There are many examples of industrial flows where both interactions are important.

Basic concepts of the present methods are very simple though various phenomena in various unit operations are calculated by the same models. Motion of individual particles is calculated numerically using the Newtonian equations of motion. As examples of simulations, various results are shown, such as hopper flows, particle segregation phenomena, particle mixing in a rotating drum, dense phase pneumatic conveying, spouted bed, dense phase fluidized bed, fast circulating fluidized bed and so on.

The discrete particle simulation has still some difficulties and several problems remain unsolved. However, even at the present premature stage, the discrete particle simulation offers results which attract attention of engineers in factories.

Peristaltic Flow of an Oldroyd-B Fluid in Channels

Siddiqui, A.
Penn State University, USA, and
Asghar, S.
University Islamabad, Pakistan

Peristaltic flows are generated by the propagation of waves along the flexible walls of a channel. Such flows play an essential role in transporting fluid inside living organisms. Many modern devices such as heart-lung machines and roller pumps have been designed on the principle of peristaltic pumping. In this paper we study peristaltic flow of an Oldroyd-B fluid in a two-dimensional channel with sinusoidal undulating walls. Because the governing equations are highly nonlinear, we use a perturbation technique to develop an analytical solution. The wavelength of the peristaltic waves is assumed to be large compared to the average half-width of the channel. Expressions of the stream function and velocity field are presented in closed form, up to and including third order terms. The pressure rise per wavelength is derived as a function of the time-average flow rate. The effects of viscoelasticity are examined through quantitative and qualitative comparisons with results obtained for peristaltic transport of Newtonian fluids. The phenomena of reflux and trapping are discussed.

A Perturbation Study of Particle Dynamics in a Plane Wake Flow

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The transport of small particles through wakes or mixing layers is a common phenomenon found in many technological and natural flow systems, with applications in such areas as power production and pollution control. The primary feature of both of these types of flowfields is their arrays of organized vortex structures. In dilute wake flows where the appropriate particle equations of motion are Lagrangian and account for drag only, a particularly interesting effect that has been observed both numerically and experimentally is "particle focusing". This refers to the tendency of particles in a certain size range to "demix" or become concentrated (i.e., focused) in narrow bands near the peripheries of the vortex structures. The origin of this focusing phenomenon is not clear, although chaotic dynamics has been the subject of some speculation.

It is the purpose of the present investigation to elucidate the nature of particle dynamics in a plane wake flow. This is accomplished by performing a perturbation analysis (in terms of Stokes number) of these dynamics in an analytically-defined model flowfield represented by a modified form of the von Karman vortex street. It is shown that there is an

attracting periodic orbit (i.e., attractor) along which particles eventually become entrained for small and intermediate Stokes numbers. This attractor undulates around the vortex cores and ceases to exist for large Stokes numbers. Focusing, which is demonstrated to occur over a range of intermediate Stokes numbers, is explained by considering centrifugal force effects in conjunction with time and length scales in the background flowfield. These are what determine the time (i.e., downstream distance) it takes for particles to spin out to the undulating attractor in the wake. Particles which spin out sufficiently rapidly within the coherent near-wake region are clearly identifiable as being focused. Those which spin out more slowly (due to a small Stokes number) reach the attractor too far downstream for any actual wake flow to remain coherent and, thus, focusing is not observed. Neither is it observed at large values of the Stokes number for which particles are ejected from the vortex street. Consequently, the focusing mechanism, which operates at intermediate values of the Stokes number only, is shown to have nothing to do with chaotic dynamics.

Modeling of Complex Two-Phase Flows Using a SPEED Model

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The Lagrangian trajectory model has been widely used to predict a variety of particulate two-phase flows [1]. The recent development of numerical methods for two-phase flows has been reviewed by Crowe et al. [2]. The conventional Lagrangian model assumes that discrete particles are interacting with a series of turbulent eddies [3]. The period of time, over which a particle is interacting with a randomly sampled eddy, is determined by minimizing an eddy lifetime and an eddy transit time. The drawback of the conventional models is that a relatively large number of particle trajectories are often necessarily tracked to achieve a stochastically significant solution, thus requiring much computer CPU time for the Lagrangian solver. To overcome this deficiency, Chen and Pereira [4-7] developed and improved *a Stochastic-Probabilistic Efficiency Enhanced Dispersion* (SPEED) model by deriving a trajectory-variance equation for the variance of particle trajectories induced by gas turbulence. The SPEED model was applied to predict different two-phase flows. It is found that the model can substantially enhance computational efficiency of the Lagrangian solver as compared to the conventional stochastic Lagrangian trajectory model. These applications are related to two-phase flows with simple geometries, and the numerical solution is based on the Cartesian coordinates. In the present work, the SPEED model is extended to curvilinear coordinates, thus making it possible to predict turbulent two-phase flows with complex geometries. The continuous fluid flow is modeled using the second-order Reynolds-stress transport model to capture the turbulence anisotropy. The partial-transformation approach that uses the Cartesian velocity vectors has been employed for the finite-volume solution to the fluid flow field in curvilinear coordinates. A robust numerical algorithm is developed to determine the probability distribution over irregular Eulerian control volumes, an essential requirement for extending the SPEED model in general coordinates. In addition, an improved particle-locating algorithm, developed by Chen [8], is developed for rapidly identifying the Eulerian control volume to which the particle has moved after each time step. The extended SPEED model is validated against experimental measurements of Sato et al. [9] for the particle dispersion in a turbulent gas flow. The main results are reported in Reference [10].

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Session: B2-2 Room: CUB B7-9 **Time:** T1:00p-3:00p
Chair: *C. T. Crowe (WSU)*

Computational Investigation on Penetration Capability of Sprinkler Sprays with Varying Parameters

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Computational models have been utilized to investigate penetration capability of sprinkler sprays directly above a fire source with respect to water flow rates, spray drop sizes, and spray momentums.

The spray models were generated by assigned representative drop size, mass flow rate, discharge speed, and discharge angle of 275 trajectories in such a way that they produced computed results match with the measured water density distribution and thrust forces in the absence of fire. The spray/fire plume interaction models were created by combining the spray models with free-burn fire plume models with a Lagrangian particle tracking scheme.

Actual delivered densities and penetration ratios were computed through the interaction simulations at six flow rates at three fire sizes under two ceiling heights. Drop sizes and spray momentums at two flow rates were increased by 25% and 50% from the original values without changing other spray characteristics and applied to three fire sizes under two ceiling heights to investigate the effects of each parameter on penetration capability separately.

The study seemed to indicate that there is an optimal flow rate for a given sprinkler that gives the highest penetration ratio within a practical flow range. It also showed that increasing drop size was much a much more reliable way for a higher penetration ratio than increasing spray momentum.

Numerical Modelling of Bubble Dynamics using a Fluid Interface Capturing Technique

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The paper presents a numerical method to predict the dynamics of bubbles, including the surface deformation, in gas/liquid two-phase flow. The numerical technique is a recent development for capturing fluid interfaces on fixed meshes (Eulerian frame). It is based on the solution by a finite-volume procedure of a transport equation for a fluid indicator function denoting the volume fraction occupied by the fluids. In contrast to the widely used VOF method which solves a similar equation, the present technique relies on a novel compressive differencing scheme to maintain sharpness of the interface at all times. The advantage of the new scheme is that not only it preserves a sharper interface than can VOF, but it also retains the shape of the interface with little deformation, a feature Which VOF is liable to produce. The method dispenses with the need for operator splitting in the different spatial directions, which is a characteristic of most if not all existing interface capturing methods. This is achieved by employing second order accurate implicit time discretisation. This feature also makes it applicable to unstructured meshes.

The method treats both phases, gas and liquid, as a single continuum obeying the same transport equations, but having different local properties depending on whether the point is occupied by one phase or the other. At the interface which is spread over two or three cells, the properties are interpolated from those of the two fluids on either side. Surface tension forces are accounted for through the introduction of a jump in pressure at the interface.

The method is applied to the simulation of the rise of bubbles in liquids; both small (but deformable) and large (Taylor) bubbles are modelled. In the calculations, the gas phase is initially introduced as a volume of arbitrary shape, since the shape of the bubble is not known in advance and is eventually determined by the flow itself. The computation proceeds to track the motion of the bubble as it rises. In order to maintain a compact domain of computation yet allowing the tracking of the bubble over a long distance, the frame of reference is attached to the bubble and is moved with it. This is accomplished automatically by sensing the speed of the bubble at every time step and imposing an opposite velocity to the surrounding liquid. In this manner the bubble is always maintained in the middle of the computational domain.

Results of the calculation for several bubble flows at different Eotvos and Morton numbers will be presented and compared with experimental data where available. Both the computed bubble shape and the rise velocity will be compared. It is shown that agreement between the calculations and measurements is excellent.

Particle-collision Induced Turbulence in Solid-Liquid Flows

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California Institute of Technology, USA

Liquid-solid flows occur in many practical applications and natural processes. The turbulence in the liquid (continuous phase) is affected by the presence of the particles (discrete phase). There is no general consensus on whether the particles enhance or reduce the turbulence levels in the fluid phase. The fluid phase itself affects the motion of the particles, enhancing or damping the fluctuating velocity components of the solid phase. The coupling between the phases in a multi-phase flow is a clear example of the complexity associated with multi-phase systems.

This study investigates the turbulence generated by particle collisions. The motion of a particle towards a wall, or towards another particle, will result in a collision if the Reynolds number of the flow is large. As the particle approaches the wall, the fluid in the gap between the particle and the wall will be displaced. When the particle touches the wall and rebounds, the direction of the flow will reverse. This process produces a considerable agitation in the fluid phase. To study this process an immersed pendulum experiment was built to produce controlled collisions of particles. A fine string is attached to a particle, which is positioned at rest from some initial angle. Once released, the particles accelerates towards a wall, or to another suspended particle, resulting in a collision. The fluid is seeded with neutrally buoyant micro-spheres, which illuminated by a laser sheet serve as flow tracers. The motion of the particles and tracers is recorded using a high speed digital camera. The images are digitally processed to calculate displacements and velocities for different times before and after the collision. Flow fields are obtained for different impact velocities, particle diameters and solid-fluid density ratios, as well as for particle-wall and particle-particle collisions.

Preliminary results show that for the flow conditions tested, the rebound of the particle is dependent on the shape of the wake behind the particle at the moment of collision, and not only on the flow in the gap between the particle and the wall. The amount of collision-generated turbulence appears to increase with impact velocity and density ratio.

Second-Order Accurate Schemes for Two-Fluid Models of Two-Phase Flow

Tiselj, I. and Petelin, S.
Jozef Stefan Institute, Slovenia

A second order accurate scheme based on high-resolution shock-capturing methods was extended to a typical two-base flow model which is used in the computer codes for simulation of nuclear power plant accidents. The two-fluid model, which has been taken from the computer code RELAP5, consists of six first-order partial differential equations that represent one-dimensional mass, momentum and energy balances for vapour and liquid. The partial differential equations are ill-posted - non-hyperbolic. The RELAP5 numerical scheme, which is based on direct discretization of the basic equations, is first order accurate and introduces a significant numerical diffusion into the solutions of the equations. Its upgrade into a second order accurate scheme is practically impossible, as numerical diffusion plays a crucial role in the stability of the scheme.

Higher order accurate numerical schemes, which allow substantial decrease of the numerical diffusion, are based on characteristic form of the basic equations. Such schemes require hyperbolic equations and explicit evaluation of eigenvalues and eigenvectors of the equations. We have developed a method for the evaluation of the eigenvalues and eigenvectors of two-fluid models and obtained the hyperbolicity by minor modification of the virtual mass term.

The basic problems of the application of second order accurate schemes on the two-fluid models are: 1) The conservative form of the two-fluid equations does not exist. 2) Numerical oscillations near the interfaces with large vapour volume fraction jumps, when equations are solved with conservative variables.

We have shown evident advantages of the second order accurate schemes especially in the area of fast transients dominated by acoustic phenomena, where equations were successfully solved using nonconservative variables. Advantages are less obvious in the area slow transients where uncertainty of the closure laws often exceeds the accuracy improvement of the second order accurate schemes.

Effect of Suction or Injection on the Periodic Flows of an Oldroyd-B Fluid

Hayat, T., Asghar, S.
Quaid-I-Azam University, Pakistan and
Siddiqui, A.M.
Pennsylvania State University, USA

The governing equations for unsteady Oldroyd-B fluid taking into account the suction/injection from the porous plate are established. The solutions of the periodic oscillations of the porous plate in Maxwell fluid are then considered. In the case of suction at the plate the solution is found to admit an asymptotically decaying behavior. However, in the case of blowing no such solution exists. This instability is because of the singularity introduced in the flow in the case of blowing which naturally does not exist in the case of suction. This provides an interesting physical insight which has also been referred in passing by Rajagopal. The results are compared and found in full agreement with those available in the literature.

The unidirectional flow of a fluid near a porous oscillating surface is of interest for two reasons: First, by virtue of its being one of those special cases for which the Navier-Stokes equations yield to exact analysis; secondly and perhaps more importantly, the decay of the amplitude of the oscillations with distance from the surface, and the effects of mass transfer on this decay, gives a quantitative basis from which the effects of mass transfer on the turbulent boundary layer can be determined. Furthermore, it is known that the understanding of fluid mechanics and heat transfer in flows with fluid injection or suction is of importance in many engineering activities.

In the literature, the solution for the oscillation of the rigid plate without suction/injection are given by Rajagopal [1] and Hayat et. al., [2]. Thus, in the sum total, we present a mathematical model of the Oldroyd-B fluid taking into consideration the suction/injection

at the porous plate. The velocity field due to arbitrary periodic oscillation of the porous plate in Maxwell model is then presented analytically. Some interesting flows caused by certain special oscillations are also obtained.

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Symposium C1
Advanced Modeling in Geomechanics and Minerals Processing
Organizer
H.-B. Mühlhaus
CSIRO, Australia

Session: C1-1 Room: CUB B11-15 **Time:** M10:00a-12:00p
Chair: *H. B. Mühlhaus (CSIRO)*

Damage Diffusion in Uniaxial Compression Of Rocks

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In this paper we put forward the microcrack buckling model by Vardoulakis and Papamichos (1991), which may be summarized as follows:

In unconfined compression of brittle solids, surface parallel microcracks buckle from the very beginning of the loading process. For small axial stresses only cracks close to the surface buckle, whereas with increasing stress deeper regions are affected. The latter may be modelled as strain-assisted damage diffusion.

Based on more recent papers by Vardoulakis et al. (1996 a,b) on stress diffusion in uniaxial compression tests on rocks and concrete, a constitutive theory of anisotropic damage diffusion is suggested. The theoretical results are used to shed some light on experimental findings pertaining to contact stress redistribution in uniaxial plane-strain tests on marble, performed on the so-called Surface Instability Detection Apparatus of Papamichos et al. (1994).

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Advanced Constitutive Relations for Geomaterials and Applications

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ALERT Geomaterials, France

Incrementally non-linear formalism describes elasto-plastic behaviours by an homogeneous of degree one non-linear relation between the incremental strain and the incremental stress. At several benchmarks workshops these relations have shown their efficiency particularly for severely non-proportional loading paths and for instabilities and bifurcations states.

However our models have two deficiencies : the too high number of constitutive parameters and the fact that the incremental strain is expressed as a function of the incremental stress (what is not convenient for finite elements computations). In this paper we propose new incrementally non-linear constitutive relations basically with 5 material constants:

$$d\varepsilon_{ij} = M_{ijkl} \cdot d\sigma_{kl} + \frac{1}{\|d\sigma\|} \cdot N_{ijklpq} \cdot d\sigma_{kl} \cdot d\sigma_{pq} \quad (1)$$

$$d\sigma_{ij} = P_{ijkl} \cdot d\varepsilon_{kl} + \frac{1}{\|d\varepsilon\|} \cdot Q_{ijklpq} \cdot d\varepsilon_{kl} \cdot d\varepsilon_{pq} \quad (2)$$

Relations (1) and (2) can be viewed as dual each other. We establish the general expressions of tensors M, N, P, Q as function of tangent mechanical characteristics.

First comparative results between models (1) and (2) are presented and discussed.

Then two kinds of applications will be considered :

1. homogeneous bifurcation points by loss of constitutive uniqueness are exhibited and post-bifurcated branches computed.
2. first finite elements computations of classical situations are finally presented.

Modelling Comminution Devices Using DEM

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CSIRO Division of Mathematical and Information Sciences, Australia

Particle size reduction, or milling, is an essential component of mineral processing and is important in other industry sectors. This needs to be done as efficiently as possible, maximising mill throughput while minimising operating costs. Such milling processes typically use only 1 to 5% of the supplied energy for particle breakage, which leaves room for improvement.

In discrete element modelling (DEM) of granular flows the trajectories, orientations and spins of all the particles and objects in the system are calculated and their interactions with other particles and with their environment are predicted. It is necessary to simulate particles of many different sizes and densities interacting with complex shaped objects moving in a range of different ways. The key ingredients are a fast and robust algorithm to predict collisions, a good collision model and an efficient and powerful method for describing the objects. The capabilities of our object oriented two dimensional DEM code and pre-processor will be described.

Particle flows in three types of mills, a 5 m ball mill, a 10 m SAG mill and a 30 cm diameter centrifugal mill are presented. Charge behaviour, torque and power draw are analysed for a range of rotation rates from 50 to 130% of the critical speed for

the ball mill. Sensitivity of the results to material properties and size distribution are examined. Ball segregation will also be discussed. Charge motion and power consumption for the SAG mill will be presented. Comparison of simulated flow patterns for the centrifugal mill with high speed experimental photographs reveals close agreement, with correct steady profiles predicted for solids loadings above 30% and qualitatively correct charge behaviour involving a three pointed structure flopping around the mill interior for lower solids loadings.

Balance Equations for the Mechanics of Poly Disperse Granular Materials

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We derive a general thermo-mechanical theory for particulate materials consisting of granules of arbitrary shape and size. The kinematics of the granulate is described within the framework of a polar continuum theory whose material points possess three translational and three independent rotational degrees of freedom. Additional field variables are the translational and rotational granular temperatures, the kinetic energies of the velocity and spin fluctuations respectively and the usual thermodynamic temperature. We distinguish between averages over particle categories (average mass/velocity and moment of inertia/spin space respectively) and particle phases where the average extends over distinct subsets of particle categories (multi phase flows). All derivations are valid for arbitrary particle shapes. Explicit expressions for the stress and couple stress tensors are derived for the case of rod-shaped particles.

Session: C1-2 Room: CUB B11-15 **Time:** M1:30p-3:30p
Chairs: *L. J. Sluys (Delft) & F. Oka (Kyoto)*

A Gradient Field Theory: Nanomechanics of Self-Organization and Localization

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There is ample experimental evidence that materials under uniform tractions evince localized deformation in the form of one or more deformation bands or of periodic deformation structures. The present work concerns itself with the depiction of localization and/or self-organization, by means of non-affine deformation fields $\mathbf{q}(\mathbf{x})$, in the context of irreversible thermodynamics. The geometric structure of these fields requires that the Helmholtz free energy density "A" or its Gibbs counterpart, be a function of the fields as well as their gradients, in opposition to the local theory where only the fields themselves appear in A.

Partial differential equations for $\mathbf{q}(\mathbf{x})$, generally non-linear, with appropriate experimentally realizable boundary conditions, are obtained in the presence of small deformation, their spatial part by invoking the global form of the dissipation inequality and their temporal part by appeal to its local counterpart. In consequence, gradient viscoelasticity is obtained when the time scale is Newtonian, gradient plasticity and viscoplasticity when the time scale is intrinsic in the sense of the endochronic theory. Non-local elasticity is a special case of viscoelasticity when the dissipation is zero.

Specific forms of the internal non-linear field equations are obtained in the light of physically dictated particle potentials that pertain to metals at room temperature. These equations are then solved numerically. Localized or periodic deformation structures in the form of single or multiple deformation bands are thereby obtained by virtue of the intrinsic non-linear material behaviour, associated with non-linear particle interactions in the form of concave/convex particle potentials. Such bands may be reversible or permanent depending on the pertaining constitutive constraints.

Of importance is the fact that the theory predicts plastic deformation by discrete particle motion (!), a phenomenon that has been conjectured on the basis of dislocation theory. Finally, necking is shown to be a particular solution leading to a central localized strain field under axial tension.

Localization Analysis of Water-Saturated Cohesive Soil

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The strain localization of a water-saturated porous cohesive soil is studied based on numerical solutions using a strain-gradient dependent viscoplastic constitutive model. Second order gradient of volumetric viscoplastic strain is introduced into constitutive model based on the Cam-clay model and over-stress type viscoplastic theory to account for the non-local effect of the motion of microstructure. The viscoplastic strain gradient dependent model is numerically studied by a finite element method (FEM) using a quadratic interpolation function for viscoplastic strain. In the FEM analysis, the Biot's two-phase mixture formulation and the updated Lagrangian scheme are used for water saturated material.

The yield function which includes a gradient term is expressed as follows.

$$f = \frac{\sqrt{2J_2}}{M^*\sigma'_m} + \ln\frac{\sigma'_m}{\sigma'_{my}} - a_3\nabla^2 v^p = 0 \qquad (1)$$

Where M^* is the stress ratio at failure, J_2 is the second invariant of the deviatoric stress tensor S_{ij} (S_{ij}=deviatoric part of σ_{ij}), σ'_m is the mean effective stress $a_3\ \nabla^2\ v^p$ is the gradient term consisting of second order gradients of viscoplastic volumetric strain and σ'_{my} is the hardening parameter.

A column specimen on saturated clay with 11cm height is sheared at a constant horizontal displacement. The weak element is introduced at the center element (Fig. 1). Numerical results with respect to the difference in the gradient term a_3 are summarized in Fig. 2. Introduction of the strain gradient term is found to work as the stabilizer in the strain localization analysis.

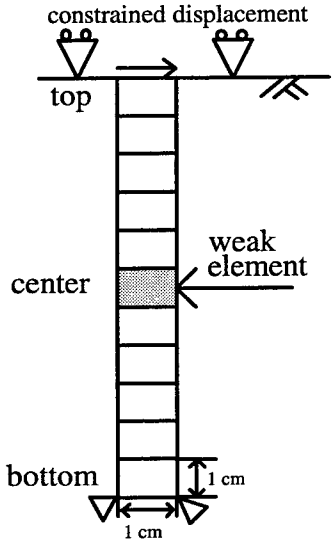
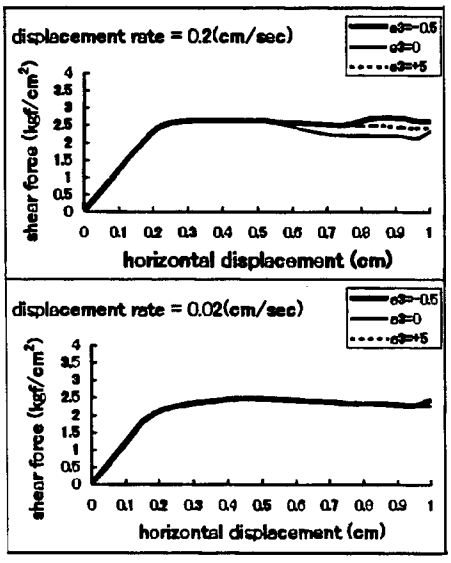


Fig. 1 Boundary Condition



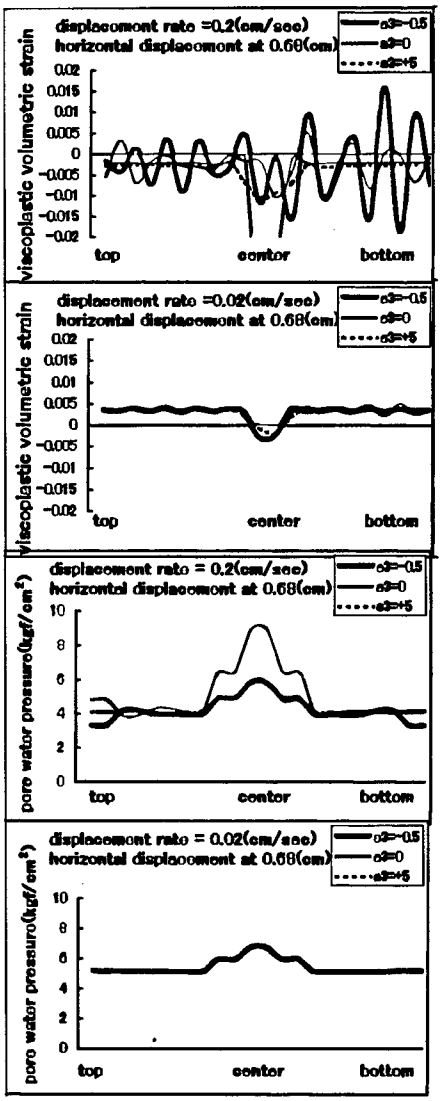


Fig. 2 Numerical Results

Shear Band Phenomena in Empty and Saturated Soils Computed by Time and Space-Adaptive Methods

Ehlers, W., Ellsiepen, P. and Volk, W.
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Shear band phenomena, as for instance the well-known slope failure or base failure problems of geotechnical engineering, occur as a result of local concentrations of plastic strains in small bands of finite width (shear bands). The mechanical reason for this behaviour lies in the basic properties of frictional materials, where, in the brittle regime, the plastic dilatation yields local softening effects. However, it is well known that the numerical description of shear band phenomena, e.g. in the framework of the finite element method, leads to an ill-posed problem. In particular, both the direction of the shear band and the shear band width itself strongly depend on the

discretization, especially, on the mesh size. For example, each mesh refinement leads to smaller shear bands until one obtains (ideally) a singular surface. To overcome this problem, two different regularization mechanisms are taken into consideration. These mechanisms are (1) the inclusion of independent degrees of freedom in the sense of the Cosserat brothers (micropolar formulation) and (2) the inclusion of pore-fluid viscosity (standard formulation). The first two regularization techniques can be successfully applied to both saturated and empty solid skeletons, whereas the last technique is restricted to the saturated case alone.

It will be shown by numerical examples that micropolarity is the much stronger tool to regularize the shear band problem than is fluid viscosity. furthermore, micropolarity includes additional material parameters (e.g. the internal length scale), which can be used for an implicit determination of the shear band width independently of the mesh size. In contrast to this, the fluid shear viscosity is a given material parameter, which can only be changed in an artificial manner to influence the shear band width. The numerical examples are based on the finite element method, where time and space adaptive methods are used both to fit the elasto-plastic skeleton behaviour together with the viscosity effect of the pore-fluid and to refine and coarsen the mesh in the near field and the far field of the localization zones.

Ehlers, W., Volk, W.: On shear band localisation phenomena of liquid-saturated granular elasto-plastic porous solid materials accounting for fluid viscosity and micropolar solid rotations. Mech. Cohesive-frictional Mater. 2 (1997), 301-320.

3d Adaptive Viscoplastic Modeling of Shear Banding

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The computational modeling of shear bands with standard rate-independent models fails because the field equations that describe the motion of the body may lose hyperbolicity in dynamics (or ellipticity in statics) when strain softening occurs. In order to solve the mesh-sensitivity problem, which is a direct consequence of this, a viscoplastic formulation of the strain-softening material is used.

This keeps the field equations hyperbolic under dynamic loading conditions and elliptic under (quasi-static) loading conditions. In many publications it has been shown that material rate dependence introduces a length scale effect into the rate boundary value problem even though the constitutive equations do not explicitly contain a parameter with the dimension of length. It was demonstrated that this viscous length scale effect can be related to the spatial attenuation of waves that have real wave speeds in the softening regime. Overstress viscoplastic methods according to Perzyna and Duvaut-Lions are successful in describing shear banding irrespective of the used finite element discretization. In this paper the so-called consistency viscoplastic model is presented in which regularization is achieved by introducing a rate-dependent yield surface. The standard Kuhn-Tucker conditions for rate-independent plasticity then still apply. A formulation with and without the inclusion of higher-order strain gradients (multiple length scales !) is discussed. The model will be explained for 2D and 3D stress situations. Simple finite elements will be used, namely for 3D 8-noded brick elements and 4-noded tetrahedral elements, both with the necessary mode enhancement to avoid locking behaviour. A delaunay-based unstructured 2D-area and 3D-volume generator has been used for mesh generation. 2D and 3D examples of mode-II failure problems will be analyzed and the main goal is to determine whether a 2D schematization of a shear band is allowed especially when the evolution of the shear band in the third direction is non-uniform and non-planar. An important issue that will be discussed in the paper is the propagation of shear bands in structured and unstructured, 2D and 3D meshes.

When a viscoplastic continuum model is used to describe shear banding very small finite elements are needed inside the shear band. This results in very inefficient meshes when the location of the shear band is not known in advance. 3D calculations of shear banding are therefore extremely time consuming. For these analyses mesh adaptation will be applied. A method that is proposed here is the Arbitrary Lagrangian Eulerian (ALE) technique by which mesh adaptation can be carried out during computation. The principle idea of the method is to decouple nodes from material particles, so that nodes can move arbitrary (i.e. independent of the material). Hence, nodes can move from the elastic part of the body inside the shear band.

A Microstructure Model for Elastic Surface Effects and Spalling

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Dames and Moore, USA

Spalling is a type of rock fracturing which occurs at free surfaces. when rock is subjected to high compressive stresses tangent to a stress-free surface, cracks form parallel to the surface breaking off thin flakes or slabs. Spalling has been observed in highly stressed boreholes, tunnels and also in uniaxial tests. Spalling in boreholes is somewhat puzzling because elastic solutions for the stress concentration around a circular hole predict that the maximum compressive stress occurs at the free surface. However, in spalling, fractures do not form at the surface, but instead form several millimeters in from the surface.

This paper explores the possible influence of elastic edge effects on spalling. When heterogeneous elastic materials (such as layered materials) are

compressed, a thin boundary layer forms at free surfaces. Within this boundary layer the compressive stress is slightly lower than that in the material farther in from the free surface. In effect, material close to a surface behaves as if it is less stiff. For the borehole problem, this means that the maximum compressive stress occurs not at the free surface, but at some small distance in from the free surface - just in the area where spalling fractures form.

To explore this elastic edge-effect theory for spalling, an elasto-plastic theory with microstructure has been developed and implemented in a finite element model. For simplicity, microstructure effects are restricted to the elastic behaviour of the material, while plastic failure and flow are expressed in terms of the classical cauchy stresses. Fracture is simulated by using strain-softening plasticity. Numerical simulations using this model suggest that the theory might be a plausible explanation for spalling in boreholes.

Session: C1-3 Room: CUB B11-15 **Time:** M4:00p-6:00p
Chairs: *E. Dawson (Dames & Moore) & H. Horii (U. of Tokyo)*

Lagrangian Particle Modelling of Silo Flows

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The mechanics of particulate materials has intrigued physicists and engineers for well over two centuries. At low strain rates, particulates such as sands or cereals behave like solids but, at high strain rates, the behaviour is fluid- or gas-like. The solid phase, governed by Hertzian contacts and frictional sliding and slow particle rearrangements is well described by the engineering theories of !soil mechanics. The transition to fluid-like behaviour, which seems to be associated with a singularity in the viscosity (glass transition), is currently not well understood at all. In the fluid-like range, the flow is accommodated by fluctuations in the particle velocities away from the mean field. This situation is very similar to the theory of dense gases and, in fact, there exists an extensive bulk of work on continuum theories for rapid granular flow that draws exactly on this similarity.

Of the currently unresolved problems in the area of continuum theories for granular materials, two in particular stand out: the crossovers between fluid-, solid- and gas- like behaviour, and a computational numerical tool capable of modelling all the complexities of granular flows. In our paper we address the latter problem. We apply a "Lagrangian Particle Method" (Sulsky and Schreyer, 1995) to the problem of free surface flow and discharge of a granular material from a silo. The granular material is assumed to be rigid-plastic, obeying the Drucker-Prager yield criterion; the effect of wall friction is included in the model.

In the Lagrangian Particle Method (LPM), one traces the position of a finite number of material points - for instance - within a finite element mesh. Within each time or loading step the position of the particles is updated based on current position, nodal point velocities, shape functions and a suitable integration procedure. Here we concentrate on slow or quasi-static flows. The particles can cross element boundaries and carry information pertinent to the deformation, chemical and thermal history depending on the nature of the problem. The stiffness equations are solved by multi-grid relaxation — a feature that makes this development particularly suitable for large-scale problems.

Micromechanics-Based Continuum Modeling for Solids with Discontinuities

Horii, H., The University of Tokyo, Japan

Mechanical behaviours of solids with discontinuities are often of great concern in engineering problems. A problem of jointed rock mass is a typical example. To find solutions to engineering problems such as design or safety assessment of a large scale cavern in jointed rock mass, the problem must be set as a well-posed mathematical problem. The number of microstructural elements involved in the problem is enormous and it is almost impossible to treat individual elements separately. Hence the original body with microstructures is replaced with an equivalent continuum. The point is how to ensure the equivalence between two problems. Micromechanics-Based Continuum (MBC) modeling provides a constitutive equation in the equivalent continuum problem by estimating the behaviour of individual microstructural element and taking average of strain and stress over a representative volume element.

Here the MBC approach for solids containing discontinuities is presented. Two examples of application of MBC modeling to rock engineering projects are presented and it is demonstrated how successfully MBC modeling answers engineering requests.

Firstly, the MBC modeling is applied to the problem of large-scale under ground excavation. The design and safety assessment of large scale excavation requires an accurate prediction of behaviours of rock masses governed by the sliding and opening of existing joints. The numerical results are compared with measured data in the excavation of underground power houses of 50m height, 30m width, and 150m length.

Secondly, the MBC model of jointed rock mass is extended for the Hot Dry Rock (HDR) projects. HDR project is to extract geothermal energy with a reservoir created by hydraulic fracturing in a deep hot dry rock. The accurate prediction of the shape and size of the fractured zone and the spatial distribution of

permeability is indispensable for the realization of HDR projects. The results of the coupled analysis for formation of fractured zone and the water flow through the opened joints are compared with field experiments conducted in different countries.

Anisotropic Hardening of Fiber-Reinforced Granular Composites

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The Johns Hopkins University, USA

Granular materials, such as soils, exhibit hardening and softening when subjected to plastic strains. The process prior to failure is characterized by an increase of stress (hardening), and the postfailure behavior is associated with a stress decrease. A number of constitutive models have been introduced to describe such a behavior. These models may be based on isotropic or anisotropic (kinematic) hardening concepts. An addition of fibers to granular media leads to an increase in the initial strength, and it also causes an additional, very distinct, hardening effect.

If the orientation of fibers is distributed uniformly, the strength of the composite is likely to be isotropic. However, a hardening effect should be expected to occur during deformation process, because of the reorientation of fibers imbedded in the composite matrix. During the deformation process the direction of largest extension becomes the preferred fiber orientation. Under plane-strain conditions, the preferred fiber orientation plane is the maximum extension plane perpendicular to the plane of deformation. Consequently, the composite becomes anisotropic, and the hardening effect needs to be classified as kinematic.

Micromechanics considerations will be shown, leading to a mathematical description of fiber reorientation during deformation processes. An influence of this fiber reorientation on the yield function of the composite will be considered. A process where the hardening effect is attributed solely to fiber orientation will be studied first. Next, both the hardening due to fiber reorientation and matrix hardening/softening will be considered. Some experimental results from triaxial testing of polyamide fiber-reinforced sand will be used to validate the description proposed.

Micro-Structure Developed in Shear Bands and its Implication in the Mechanics Of Granular Media

Oda, M. and Iwashita, K.
Saitama University, Japan

Micro-structural changes which took place in shear bands of five natural sands were observed by means of a microscope and thin sections, with special interest in their implication in the mechanics of granular media. The results are summarized as follows: 1) Extremely large voids are produced in shear bands, and the resulting void ratio can be larger than a maximum void ratio. 2) Particle orientation changes sharply at shear band boundaries so that a high gradient of particle rotation can be developed within a relatively narrow zone during the shear banding process. 3) In the strain hardening process, the main micro-structural change is the development of column-like structure extending parallel to a major principal stress direction. The columns start buckling at a peak stress, and the buckling columns tend to concentrate in shear bands during the strain softening process, which causes not only the growth of the extremely large voids but also the particle rotation in shear bands. These observations suggest that 4) rotational stiffness at contacts must be one of the important components controlling the strength of granular soils.

Numerical tests were carried out to simulate the micro-structure developed in shear bands, as well as overall stress-strain behavior of granular soils. To do this, the conventional distinct element method (DEM) was modified a little such that the effect of the moment transmission through contacts can be taken into account. The results are summarized as follows: 5) The development of shear bands can well be simulated only when the moment transmission is considered in DEM. Not only the generation of large voids but also the particle rotation in the shear bands can both be reproduced, in a quite similar manner to those of the natural granular soils. 6) Column-like structure (column) is well developed in DEM, regardless of whether the moment transmission is considered or not. 8) Couple stress is generated, at an appreciable amount, in a consistent manner with the result based on the micropolar-continuum theory. 9) Stress can be discontinuous along the shear band boundaries.

From the experimental and numerical studies, two conclusions were obtained: Rotational stiffness at contacts plays a key role in generating the micro-structure (large voids and particle rotation) observed in shear bands. Micro-polar continuum theory might have a chance to provide a theoretical basis for a bifurcation analysis of granular media.

Localization Analysis by the Subloading Surface Model with a tangential Stress Rate Effect

Hashiguchi, K.
Kyushu University, Japan

The localisation phenomena is analysed by the noncoaxial subloading surface model with tangential stress rate effect. Plastic stretching is independent of the stress rate component tangential to the yield or loading surface, called the tangential stress rate, in the traditional elastoplastic constitutive equation with a single and smooth plastic potential surface. It leads to the coaxiality, i.e. principal directions of plastic stretching coincides with those of stress. For metals the

single crystal grains have multi-slip system and thus the inelastic stretching would be dependent of the tangential stress rate, however. They may be observed to some extent even for a polycrystalline metals in which an infinite number of slip systems are activated, because some single crystal grains in the material influence the deformation behavior in terms of macroscopic viewpoint. They cannot be neglected in the process that the loading path abruptly changes or deviates severely from the proportional loading as observed in the plastic instability phenomena with a localization of deformation. The extension of the constitutive equation so as to describe the dependency of inelastic stretching on the tangential stress rate would be one of the most fundamental but unsolved problems in elastoplasticity at present. Therefore, various models for this aim have been proposed as was reviewed in detail in the previous article (Hashiguchi, 1997).

In this article, the elastoplastic constitutive equation is extended so as to describe the non-coaxiality of a stress and an inelastic stretching by introducing a novel para-inelastic stretching caused by the tangential stress rate, generalising the Rudnicki and Rice's (1975) J2-deformation theory in the rate form and incorporating it into the subloading surface model (Hashiguchi and Ueno, 1977, Hashiguchi, 1980, 1989) with a smooth elastic-plastic transition. It fulfils the mechanical requirements, i. e. the continuity condition, the smoothness condition, the work rate-stiffness relaxation and the Masing effect (Hashiguchi, 1993a) would be a pertinent inelastic constitutive equation applicable to an arbitrary loading process including unloading, reloading and reverse loading processes, unlimited to the proportional loading process. Based on this equation, the constitutive equation of metals with the isotropic-kinematic hardening is formulated.

Session: C1-4 Room: CUB B11-15 **Time:** T9:30a-11:30a
Chairs: ***P. Hahres & N. D. Cristeseu***

Complex Dynamics of a Creep–Slip Model of Earthquake Faults

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The classical spring–block model by Burridge and Knopoff (BK) is generalized in order to account for the irreversible deformation (creep) of the fault interface in addition to rigid sliding displacements. By this generalization the driving forces are allowed to relax, and a rate- and state dependent friction with velocity-softening is introduced. The model exhibits a new kind of short-wavelength instability that is associated to microfissuration during a seismic creep and by means of which parts of the fault self-organize to the critical state defined by the onset of velocity softening. The model is discussed in relation to the BK model (where this type of instability is absent) and compared to threshold models exhibiting self-organized criticality. Numerical results show intermittency of the seismic cycle and give power-law scaling of the event-size distributions. The implications of the model are that whereas the main shock may not be predictable, aftershocks which in some cases are equally damaging, may be.

Plastic Waves in Granular Soils

Osinov, V.
University of Karlsruhe, Germany

Granular soils are know to exhibit inelastic behaviour when subjected to large deformation. This necessitates the use of a plasticity model to describe their mechanical behaviour. In the present paper a theoretical investigation of large-amplitude waves in granular soils is presented.

The mathematical model is based on the hypoplasticity theory for granular materials. The hypoplastic constitutive equation models such features of granular materials as dilatancy and contractancy, critical states, pressure dependence and density dependence of stiffness including hysteresis. The parameters of Karlsruhe sand are used for numerical calculations. Waves in dry, partially saturated and fully saturated bodies are considered. In the case of partial saturation confined compressibility of the medium due to the presence of gas bubbles is taken into account.

The range of the wave speeds is calculated as slopes of characteristics of the system of dynamic equations. It is shown that under certain conditions the dynamic equations can lose hyperbolicity and the initial boundary value problem can thus become ill-posed. In a fully saturated body this leads to the loss of stability of the static equilibrium and to a spontaneous collapse. Numerical solutions for plane and spherical waves are obtained. In a dry or partially saturated body transverse and longitudinal types of motion are coupled through dilatancy and contractancy of granular material.

Transverse and longitudinal waves can exist separately only under specific conditions. Transverse periodic disturbance on the boundary of a half-space induces longitudinal oscillation of the inner points with double frequency.

Optimistic/Pessimistic Behaviours of Heterogeneous Body with Statistically Varying Material Properties

Hori, M. and Munashinghe, H.S.
University of Tokyo, Japan

In general, geo-materials such as soil or rock is highly heterogeneous, and the geological structure often changes abruptly. This causes a serious problem when behaviours of geo-structures or crust are

analyzed, since it is not possible to use the exact properties and structure in the analysis. The perturbation analysis (such as used in a stochastic finite element method) may not be suitable when the variance of the heterogeneity are large.

For the analysis of such a heterogeneous body, this paper proposes a new treatment. If some statistical data for the heterogeneity are given, two fictitious bodies are rigorously defined such that they yield optimistic and pessimistic evaluation for the expected behaviour. The definition of the body is based on the generalized Hashin-Shtrikman variational principle, which provide two approximate solutions bounding the exact solution of a boundary value problem for a general heterogeneous body.

It is shown that the two bodies defined from the statistical data actually produce the optimistic and pessimistic behaviours of the expectation which is computed by using Monte-Carlo simulation. Results of some other illustrative problems are shown.

1. S. Namat-Nasser and M. Hori (1993), Micromechanics: Overall Properties of Heterogeneous Materials, Elsevier.
2. H.S. Munashighe, M. Hori and Y. Enoki (1996), Application of Hashin-Shtrikman Variational Principles for Computing Upper and Lower Approximate Solutions of Elasto-Plastic Problems, Int. Con. On Urban Eng. In Asian Cities in the 21st Century, 1.
3. M. Hori and S. Sunil (1997), Two Approximate Solutions Bounding Exact Solution of Heterogeneous Body Problem (to be submitted).

Compaction and Gravitational Creep Flow of Granular Materials

Cristescu, N.D., Cazacu, O. and Cristescu, C.
University of Florida, USA

We consider the creep flow on slopes of earth, sand, mud, volcanic lava or granular materials (or pastes) used in a variety of industries.

First the slow compaction in time of a granular material deposited on an inclined plane is studied. For this purpose a nonassociated viscoplastic constitutive equation is used. It is shown that by gravitational compaction, the density increases with depth. Thus, the flow properties will also vary with depth. We discuss, for instance, how the yield stress may vary with density (with depth) and as such change the yielding properties. Further we study the increase of the shearing stresses as the thickness of the layer is increasing. We show at what depth is the shearing occurring for the first time and how the layer which is shearing may enlarge. In the general case there is a layer at the top of the stratum which remain rigid, but in motion, during shearing sliding. Also, at the bottom there is a layer which remain rigid and at rest. We show also that the bottom layer may slide along the bottom surface if a certain friction condition exists there. We discuss when such sliding is possible and the consequence on the whole shear motion. The incipient motion of the granular strata is described.

Discrete Element Modelling of Liquefaction in Calcareous Sand

Sakaguchi, H. and Mühlhaus, H-B.
CSIRO, Australia

Discrete element modelling eliminates the need for complete finite element meshes and is very well suited for micromechanical studies of granular materials. Here we put special emphasis on granulates with varying particles shapes and sizes. We present a model and applications for coupled pore fluid and particle deformation within the context of liquefaction problems. In the simulation rod-shaped macroparticles are used to model the influence of the shape, deformation, and crushing of particles on the overall response of the sample. Using this model, we have simulated cyclic simple shear tests for water saturated calcareous sands. The results are in satisfactory agreement with what is observed in physical experiments for certain calcareous sands. Note that bending and buckling behaviour which may cause the particle fracture process are typical for the rod-like macroparticles and would not occur in connection with the simulation using spherical particles.

Symposium C2
Computational Methods for Granular Materials.
Organizers
B. Loret
Institut de Mecanique de Grenoble, France
&
M. Mehrabadi,
Tulane University, USA

Session: C2-1 Room: CUB B11-15 **Time:** T1:00p-3:00p
Chairs: *B. Loret & M. Mehrabadi*

Fluid/Particle Interaction in Simulations of Granular Material

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The numerical simulation of granular material is a computational tool that is well established and widely used. However, many applications require a coupling between solid particles and a fluid: for example, the flow of groundwater in soil or the erosion and transport of particles from a stream bed. The type of formulation that is used to represent solid/fluid interaction depends on the nature of the system being modeled. At one extreme, it may be adequate to include only one-way interaction, when particles are influenced by the fluid motion, but the fluid is not affected by the particles. At the other extreme, simulation of the full process of interaction is necessary, when there is strong and nonlinear coupling between the two phases. A review is made of the spectrum of mechanisms that occur when fluid and particles interact. Then, techniques for representing these mechanisms are described, including the use of particles to model both the fluid as well as the solid objects. Finally, several applications involving fluid/particle interaction are presented. The examples range from oil flow through an assembly of proppant particles in a packed fracture to dynamic gas-solid interaction resulting from the detonation of high explosive.

Numerical Simulation of Large Shear Deformation in Granular Material

Bardenhagen, S.G., Brackhill, J.U.
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Sulsky, D.L.
University of New Mexico, USA

Numerical simulations of granular material undergoing large shear deformation are performed. The simulations are on the scale of the grains, and are designed to provide insight into the nature of the deformation at the microscale. The role of a weak interstitial material is examined by simulating both dry granular materials (no interstitial material) and approximations to plastic-bonded explosives (PBX's).

The particle-in-cell code FLIP, a computational technique employing a mix of Eulerian and Lagrangian approaches, provides a robust treatment of large deformation problems. Constituent interactions include bonding and frictional contact. The simulations are performed in 2-D and the geometry is chosen to approximate that found in a particular PBX composed of 95% by weight energetic crystals and 5% binder. Two distinct phenomena are observed. Granular "locking" occurs intermittently during the shearing when the deformation cannot be accommodated by grain rotation and translation. In these cases a small percentage of the grains are significantly stressed as the load is concentrated in chains. This phenomenon is known as stress bridging. After sufficient straining, shear banding is observed. A weak zone develops in the material after which deformation is concentrated in a region a few particles wide. Both locking and shear banding have been observed in dry granular materials. The computations predict that they will also be found in PBX's.

It is expected that these results in 2-D will be confirmed by calculations in 3-D, but 3-D simulations are clearly needed. In particular, the geometry can only be accurately represented in three dimensions. This study constitutes a first step in the coupled mechanical/chemical modeling of initiation in PBX's.

Granular Dynamics Simulation

Loret, B., Prevost, J.H.
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Tantalla, J.
Princeton University, USA

A two dimensional granular dynamics simulation was developed based upon the discrete element method and the rigid body impact method. Specifically, for the rigid body impact assumption, the Poisson restitution hypothesis with Coulomb friction has been implemented. The model leads to an implicit set of equations. A methodology for solving the simultaneous impact of multiple bodies was developed and is analyzed. Explicit direct integration is used for the discrete element model. Newton Raphson, memoryless conjugate gradient, and Gauss Seidel solvers were implemented, and a comparison of the efficiencies of the various solvers has been performed. Accurate time step estimates are discussed. A number of test cases, involving many particles, are presented to demonstrate these efficiencies.

Simulation of Two Dimensional Fluid Flow in Soils

Masad, E.
Turner Fairbank Highway Research Center, USA
and Muhunthan, B.
Washington State University, USA

A program for simulation of two-dimensional fluid flow in a saturated anisotropic soil medium is presented. The proposed program effects a numerical solution to the complete set of Navier-Stokes equations at the soil microstructural level without *a priori* assumptions on the viscous or convection components. Therefore, the solution is not restricted to a certain range of material porosity. The flow field is calculated within actual images for three granular materials that differ in porosity, particle size, and shape. Periodic boundary conditions are imposed along the border of the images.

The permeability tensor coefficients of the soil medium are derived from the computed flow fields. The numerical values of permeability and permeability anisotropy ratio compared favorably with laboratory and field experimental data. The permeability prediction can be further improved by increasing the image resolution to capture the actual specific surface. The permeability anisotropy was found to be correlated with particle elongation.

Session: C2-2 Room: CUB B11-15 **Time:** T3:30p-5:30p
Chairs: *M. Oda (Saitama U.) &*
A. Anandarajah (Johns Hopkins U.)

Numerical Model for Nonlinear Self-Weight Consolidation

Papanicolaou, A.N., Muhunthan, B.
Washington State University, USA and
Diplas, P.
Virginia Polytechnic Institute and State University, USA

The self-weight consolidation process of solids is of importance in many fields of applied sciences. This paper presents a model, which accounts for the non-linear physical phenomena underlying this process. The governing equation is a non-linear second order transient partial differential equation of the parabolic type with the effective stress as the dependent variable. The model can describe the consolidation process for a wide range of materials. The finite element and finite difference formulations were used to provide a numerical solution to the governing equation. The results are shown to be in good agreement with available experimental consolidation results on attapulgite and kaolin. Comparison with the linear consolidation models show that their predictions to widely differ from experimental data.

Simulation of Micro-Changes in a System of Particles in Silos during Filling

Gavrilov, D. and Vinogradov, O.G.
University of Calgary, Canada

The process of filling a silo with particles is simulated by placing them one-by-one at random locations. In simulations, a plane problem is considered and the particles are represented by disks. After each disk is placed on the system of disks already in a silo, the distribution of normal and shear stresses is recalculated. If any shear stress exceeds the predetermined limit, a slip takes place. Also, if a normal stress becomes tensile, it is set to zero, i.e. the two disks become disengaged at this interface. Thus the system of particles undergoes topological changes in the process of loading. Such changes in the system are handled by a Recursive Inverse Matrix Algorithm (RIMA) which allows efficient addition/removal of contact interfaces between the particles by updating the inverse matrix of the system rather then generating and solving a system of equations after each topological change. It is found that the micro-changes in topology may result in macro-effects, such as local avalanches. The extent of such instabilities is determined numerically using RIMA update algorithm iteratively. As a result of irreversible events taking place during the filling operation, the final stress state in a filled silo is loading history-dependent. A numerical example of filling a silo with 500 particles will be given as an illustration.

Numerical Analysis of Higher-Order Continua in Description of Granular Assemblies

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Internal structure of the granular assemblies - in contrast to the cemented, concrete-like materials- show a high variability under external mechanical effects. Grains may slide or roll along each other, contacting grains may be separated or new contacts created, slip lines and local collapses may occur, etc. The classical theories based on traditional continuum-mechanics often turn out to be unreliable in the description of this material whose most important feature is that it is *not continuous* at all: instead, it has a very characteristic internal structure that strongly influences the macro-level behavior. Phenomena related to volume changes or grain rotations are often mentioned as features that traditional theories cannot properly reflect.

Application of higher-order continua with multiple degrees of freedom could perhaps be a powerful tool in the theoretical modeling of granular assemblies. Our recent researches focus on the comparison of continua and granular assemblies, with the help of numerical simulations. Experiments showed that the state variables of traditional continuum-mechanics may not

contain enough information; significance of grain rotations was directly pointed out by specific tests; and the shear behavior of granular assemblies was compared to the behavior of higher-order continua. The presentation will introduce experiments and discuss their results.

Study on Elastoplastic Behavior of Granular Model in Terms of Two Dimensional Numerical Tests

Kishino, Y.
Tohoku University, Japan

This paper discusses the constitutive model for granular materials in terms of two dimensional simulation of element tests. The numerical simulation, which is carried out by the granular element method proposed by Kishino, consists of two parts; monotonic loading tests along several loading directions and probe tests to study incremental behaviors at each loading step. All the numerical tests were performed under stress-control condition. The extent of elasticity and plasticity is specified by the incremental loading and successive unloading in the direction of each probe test. The results of probe tests before the transition point, at which the strain increases suddenly, supports the elasto-plastic model. Namely, the incremental behavior can be described in terms of the incremental elastic compliance for the elastic part and the flow rule for the plastic part. However, as for the latter part, the non-associated flow and the non-coaxiality between stress and incremental strain are obtained. The observation of incremental displacement fields in the probe tests leads to the conclusion that the flow rule stems from a special deformation mode which is common among all the probe tests in which the plastic deformation occur. This conclusion is also verified in terms of a parameter of heterogeneity in the incremental displacement field which is called the deformation covariance tensor.

Modeling Split Hopkinson Pressure Bar Tests with a Discrete Element Method

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Daudeville, L. and Davenne, L.
ENS Cachan/University, Canada

In order to study the behavior of materials under strong impact loading, Split Hopkinson Pressure Bar tests were carried out on concrete specimens. These are analyzed with a Discrete Element Method. This method is particularly well adapted to problems involving fracturing and fragmentation in geomaterials because it is based on a discontinuous description of the medium. The material is represented by an assembly of rigid spherical elements which obey Newton's law of motion and interact with brittle-elastic forces. A Mohr-Coulomb type rupture criterion is given for the links between elements. As the cohesion between interacting elements vanishes, a Coulomb friction is used to simulate new contacts. The concrete specimen is modeled as a 3D cylindrical assembly of discrete elements for which the physical properties are calibrated in terms of the real sample macroscopic properties. These include density, elasticity and strength parameters. The simulations input data are the recorded input and output velocities of the laboratory experiments. The simulations output data are the computed input and output force to be compared with the experimental input and output force data. If the model behavior is correct then the misfit between the observed and the computed data should be minimum. This is repeated for three different loading rates. Despite the inherent difficulties of obtaining a comparable laboratory data set due to the extremely short time interval in which the process takes place, there is a rather good fit between the model and the experimental data. This is true, although, no viscosity was used in the model which suggests that the strain-rate dependency of fractures in concrete is more a structural (inertial) effect than a material effect (viscosity).

Session: C2-3 Room: CUB B11-15 **Time:** W9:30a-11:30a
Chairs: *Y. Kishino (Tohoku U.) & J. Dvorkin (Stanford U.)*

Efficient Algorithm of Contact Detection for Ellipsoidal and Spheroidal Discrete Elements

Sawada, S.
Kyoto University, Japan

Recently many numerical results using ellipsoidal discrete element have been reported for analyzing behavior of granular materials. Several methods of contact detection for ellipsoidal discrete elements have been developed. Those methods are based on the solution of two ellipsoidal equations. It is very difficult to solve the equation efficiently.

A new method of contact detection for ellipsoidal discrete elements is proposed. The method is developed from the geometrical point of view. In this method, iterative calculation, which is necessary to decide the contact plane, is done efficiently by the bisection method because the range of solution is easily predicted. By this calculation, the contact detection of two ellipsoidal element is converted to the contact detection of two circles, and consequently the contact forces which are calculated after the contact detection are easily defined. The contact detection of the ellipsoidal element and plane wall does not require the iterative calculation.

The method is applied to the three dimensional spherical discrete elements. Only once iterative calculation is necessary to decide the contact plane even in the three dimension. The contact detection of

two spheroidal elements is converted to the contact detection of two spheres by this method.

Several numerical examples of the plane-strain bi-axial compression tests are also shown. Ellipsoidal elements with different flatness ratio has been used for the simulations of compression test under constant strain velocity condition. Anisotropy in the strength and deformation of an assembly of particles with different shapes has been discussed from the simulations data together with the laboratory data. It is found that this numerical method using ellipsoidal elements could simulate the shear behavior and anisotropy of a sand to some extent.

Effects of Particle Shapes on DEM-Simulated Behavior of Granular Materials

Rothenburg, L. and Ouadfel, H.
University of Waterloo, Canada

The paper will focus on qualitative and quantitative features of numerical experiments with particles of different shapes and dimensionality: disks, elliptical and polygonal particles in 2D as well as of 3D spheres and ellipsoids. Results of a large number of simulations carried out over several years will be summarized to present a consistent pattern of particle shape influence on shear strength and deformation properties of granular assemblies. Simulations to be discussed include biaxial compression tests on 2D particles and triaxial/true triaxial test on 3D systems.

Most physical effects that are observed in assemblies of non-circular/non - spherical particles are in one way or another associated with particle rotations. In experiments that involve compaction of particulate assemblies, very high densities are achieved due to the tendencies of eccentric and angular particles to rotate and fill voids. At the same time, during simulated shear tests, eccentric and angular particles rotate in such a way as to preserve interparticle contacts and to delay failure. In the post-failure range, softening is much more gradual compared to assemblies of disks and spheres. These qualitative conclusions apply to particles of moderate eccentricity. Very elongated particles, on the other hand, exhibit an opposite trend when rotations become overly disruptive and affect density and strength negatively. Similar trends are observed in 2D and 3D systems.

On the analytical side, the paper will concentrate on means of characterizing mechanical response of granular assemblies in terms of macroscopic tensors describing evolution of anisotropy in orientations of intergranular contacts and contact forces. An analytical relationship between the stress tensor and microstructure tensors, the so-called stress-force-fabric relationship, will be discussed in a variety of formats and its accuracy demonstrated based on results of simulations.

Adaptative Dynamic Relaxation for Granular Mechanics

Bardet, J-P.
University of Southern California, USA

The first discrete modeling of granular assemblies coincides approximately with the development of computers in the 1970's (e.g., Cundall and Strack, 1978). Since then, researchers have realized the power of computer simulations to understand the mechanics of granular materials. These simulations generate abundant information on particle displacements, contact forces and other physical quantities, which can be processed rapidly to comprehend the mechanics of granular assemblages.

The main emphasis of our presentation is to review a basic computational technique – dynamic relaxation – in granular mechanics and to unveil its advantages and potential misuses. Dynamic relaxation, which is conveniently abbreviated as DR, consists of finding a static solution by using a dynamic transient analysis method. Reviewed in Underwood (1983), DR has been applied to various types of problems in nonlinear structural analysis. DR uses the central difference algorithm. Papadrakakis (1981) and Underwood (1983) optimized the DR parameters (i.e., mass matrix and damping coefficient) by developing adaptative dynamic relaxation techniques (ADR). One of these ADR techniques was applied in Bardet and Proubet (1991) to granular assemblies. We will present some of the most recent developments and applications of ADR (Bardet, 1998).

Bardet, J.P., 1998, Introduction to Computational Granular Mechanics, in Mechanics of Granular Media, B. Cambou, ed., CISM Courses and Lectures, Springer-Verlag, Vienna, Austria, in press.

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Papadrakakis, M., 1981, A method for the automatic evaluation of the dynamic relaxation parameters, Computer methods in applied mechanics and engineering, 25, 35-48.

A New Approach to Discrete Element Modeling

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US Army Cold Regions Research and Engineering Laboratory, USA

Current two-dimensional discrete element models use disks and polygons, while three-dimensional models use spheres and polyhedra. Since disks and spheres are symmetric establishing whether or not two particles are in contact is trivial. To do the same with polygons and polyhedra is a complicated exercise in computational geometry. I propose a new approach to discrete element modeling using a new class of objects. The class of objects may be defined as having a surface which is equidistant from a constraining point, line, surface, or solid. For example, a sphere is defined by a surface which is equidistant from a point. An infinite cylinder is defined by a surface which is equidistant from an infinite straight line. If the line is finite then the cylinder will have hemispherical ends. A torus is defined by a surface which is equidistant from a circular line. A circular disk with a semi-circular edge is defined by a surface which is equidistant from a circle. A polygonal disk with a semi-circular edge is defined by a surface which is equidistant from a plane polygon. And so on. Since each of these objects shares the common property of equidistance from a constraint point, line or surface, the same contact detection strategy applies to each. Because of this they may coexist in the same simulation. Broadly speaking there is no analytical way to determine when any two objects belonging to this class are in contact. There is however a simple and intuitive iterative approach which can detect contact.

Particle Rotation and Couple Stress in Numerical Simulations by Distinct Element Method

Iwashita, K. and Oda, M.
Saitama University, Japan

Based on the observation of micro-structure changes in shear bands of natural sands, Oda and Kazama (1998) have shown that that a high gradient of particle rotation is one of the characteristic features developed in the shear bands. If the gradient of particle rotation is introduced as an independent strain measure, then an additional stress-like quantity, called the couple stress, is required to formulate a complete set of equations. Unfortunately, however, there existed no direct experimental evidences supporting couple stress so far. Numerical analyses were carried out using the distinct element method (DEM) with great interest in the generation of couple stress inside a shear band. To do this, the conventional DEM was modified such that the effect of rolling resistance at contacts can be taken into account (MDEM). Then a central portion around a clear shear band was divided into ten square bands, named the bands 1 to 10, which are all parallel to the shear band boundaries. The average stress and couple stress were calculated by using contact moments and contact forces acting on particles belonging to each band, with the following conclusions:

1) Couple stress acting on a plane parallel to the shear band boundaries changes significantly from the bands 1 to 10. Large couple stresses are working in the bands 6 and 7, as compared with the bands 1 and 10 which are located outside the shear band. More importantly, the sign of the couple stress changes from negative in the band 6 to positive in the band 7, in a consistent manner with the result obtained from the micropolar-continuum theory by Tejchman (1997). We also observed the non-symmetry of stress tensor; i.e., . However the difference is very small.

2) Mohr stress circles were depicted to see the stress state in each band. In the bands located outside a shear band, the major and minor stresses almost coincide with the stresses applied to the boundaries of the assembly, and their principal directions are more or less parallel to the vertical and horizontal directions, respectively. The stress inside the shear band yields much smaller stress circles with the major principal stress axis in the directions inclined to the vertical at about 20 degrees. The detail analysis strongly suggests that the stress jumps discontinuously between the outside and inside of a shear band.

Oda, M. & Kazama, H. (1998). Micro-structure of shear band and its relation to the mechanisms of dilatancy and failure of dense granular soils. G*otechnique, (in printing).

Tejchman, J. (1997). Personal communication.

Session: C2-4 Room: CUB B11-15 **Time:** W1:00p-3:00p
Chairs: *L. Rothenburg (U. Waterloo) &*
B. Loret (Inst. De Mech. De Grenoble)

Deformation Mechanisms in Granular Materials

Kuhn, M.R.
University of Portland, USA

The paper presents the results of numerical experiments on large dense assemblies of two-dimensional circular particles. A technique was used to measure and observe deformation at the smallest possible scale of individual particle clusters. Measurements were made of velocity gradients within void cells and the contributions of individual contact movements to the overall deformation. These methods allowed for direct visual observation of deformation on a micro-scale. The predominant observed deformation structure was in the form of narrow "microbands," within which intense slip deformation occurred. The microbands have thicknesses of two to four particle diameters and are separated by as many as a dozen particle diameters. Significantly, these bands formed spontaneously at very small strains, well before the

onset of significant plastic deformation, and they persisted even after the peak stress was attained. Although somewhat sinuous, the microbands were roughly linear structures, oriented oblique to the principal stretch directions. Two sets of bands were observed, corresponding to two slip directions that were symmetric with respect to the major principal stretch direction. As deformation proceeded, the bands became slightly more parallel with the major principal stretch direction. Microbands are not static structures--they were found to shift, disappear, and emerge as the material was deformed. Simple shear deformation occurred within the bands, but no intense dilation was found to occur in directions normal to the bands. The bands were primarily an expression of the tangential contact motions between particles. Deformation and energy dissipation were concentrated within the microbands. Just as contact "force chains" may be considered the predominant expression of stress at the micro-scale, microbands appear to be the predominant deformation mechanism at a micro-scale. Although they are very complex structures, microbands are likely essential to the understanding of deformation in dense granular materials. The paper discusses these and related observations.

A Network Model for Powder Densification During Initial Stage Sintering

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Cypress Semiconductor, USA
McMeeking, R.M.
University of California, Santa Barbara, USA

A network model is used to simulate the sintering of crystalline powders. In these simulations every particle center is represented by a node and every contact between neighboring particles by a discrete element. The velocity of each node is related to the applied and sintering forces based on the active deformation mechanisms. These mechanisms are controlled by grain boundary and surface diffusion and they determine the constitutive laws for the behavior of each discrete element. The contribution of each discrete element is then assembled into a system of equations that represent the behavior of the powder system. Solution of these equations provides a mechanism-based study of sintering.

Macroscopic behavior of powders during sintering is characterized in the form of an isotropic constitutive law. Network modeling is allows us to evaluate sintering stress, bulk and shear viscosities, parameters of the constitutive law, in a physical simulation. This involves the application of a dilatation and simple shear rate to the exterior particles of the compact and allowing the interior particles to remain free except for the constraint imposed by the neighboring particles. Predicted values of the bulk and shear viscosities are between the upper and the lower bounds predicted by other available models. Prediction of an almost constant value for sintering stress, on the order of the ratio of surface energy to particle radius, is in good agreement with the experimental results.

Sintering of crystalline powders containing rigid inclusions is studied. The simulation results are compared with the experimental results. Densification of a powder compact, which is porous inside and dense outside, is also simulated and initiation of a crack at the boundary of porous region is predicted. Densification of initial sintering of copper and zirconia powders has been investigated. Results show that a compact of same size zirconia powder particles reaches their equilibrium configuration at a lower density than a compact of copper powder.

In practical cases, powders further densify due to the coarsening process. Therefore formulations are developed for the sintering and coarsening of rows of unequal size spherical particles through variational principle and extremization of an energy functional. Free and pressure assisted sintering and coarsening of rows of particles is investigated by numerical treatment of the formulations. Effect of initial sizes, dihedral angle, diffusivities, and compressive forces are investigated.

Mechanics and Physics of Clean and Contaminated Clays

Anandarajah, A.
The Johns Hopkins University, USA

Essential to the development of mathematical relations to describe the stress-strain behavior, shear strength and flow properties of a soil is thorough understanding of the mechanics and physics of particle-to-particle and particle-to-fluid interactions. In a fine-grained soil, in addition to mechanical interparticle interactions as in a granular material, there are physico-chemical interparticle interactions, which depend not only on clay mineralogy and microfabric, but also on composition of interstitial pore fluid. As a result, when a clean (i.e., water-saturated) clay becomes contaminated with, say, a fluid such as benzene, the mechanics and physics change, leading to possible alterations of engineering properties, some of which, if not properly accounted for, may prove to be disastrous. In this talk, the mechanics and physics of a saturated clay will be discussed, with special attention to the interparticle physico-chemical forces including the double-layer repulsive and van der Waals attractive forces. A numerical simulation procedure based on a method known as the discrete element method, which is similar to the molecular dynamics method but applied at the particle level, has been developed and used to aid in the fundamental studies; some results will be presented and discussed.

Anandarajah, A. and Chen, J., "Single Correction Function for Retarded van der Waals Attraction," J. Colloid Interface Sci., Vol. 176. No. 2, 1995, pp. 293-300.

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Anandarajah, A. and Chen, J., "Double-Layer Repulsive Force Between Two Inclined Platy Particles According to Gouy-Chapman Theory," Journal of Colloid and Interface Science, Vol. 168, 1994, pp. 111-117.

Anandarajah, A., "Discrete Element Method for Simulating Behavior of Cohesive Soils," Journal of Geotechnical Engineering Division, ASCE, Vol. 120, No. 9, 1994, pp. 1593-1615.

Two Practical Problems of Particulate Mechanics

Dvorkin, J.P. and Bachrach, R.
Stanford University, USA

Unconsolidated sands present an important exploration target for oil and gas. They are abundant in such strategically crucial oil provinces as the Gulf of Mexico and the North Sea. Such sands also constitute many shallow environmentally important aquifers. The tool most commonly used for delineating such sands and determining the type of pore fluid is seismic. P- and S-wave velocities obtained from seismic experiments can be used for characterizing the subsurface regions of interest. In order to quantitatively interpret the elastic wave velocities, one has to forward model the elastic properties of a sand-like particulate material depending on its porosity, elastic constants of the grains, and the compressibility of the pore fluid. We find that the Hertz-Mindlin contact model combined with the mean-field approximation and corrected for porosity gives accurate estimates to the bulk and shear moduli of the aggregate's dry frame as measured in seismic and acoustic experiments. However, this model appears to be satisfactory only for aggregates subject to confining pressure of more than 5 MPa (approximately 500 m of burial). It largely overestimates the elastic moduli of shallow (about 5 m of burial) sand. Another problem is that the model (although giving adequate estimates for the bulk and shear moduli) overestimates the Poison's ratio by an order of magnitude at all pressures.

Our analyses suggest that:

(a) The elastic moduli at a low confining pressure may be overestimated by the Hertz-Mindlin model due to the angularity of sand grains. Specifically, due to angularity, the contact radius between the grains is much smaller than their actual radius. This fact results in a strong reduction of the normal and shear contact stiffnesses between the grains. This angularity factor is engaged only at low pressures since sands re-pack and the raggedness of the grains decrease due to compaction.

(b) The mismatch between the theoretical and observed Poisson's ratio may be due to reduced tangential stiffnesses at some grain contacts which, in turn, may result from the presence of lubrication (e.g., water or clay) or the heterogeneity of stress distribution in the aggregate.

Time-Dependent-Subloading Surface Model

Hashiguchi, K.
Kyushu University, Japan

The deformation which depends on a time is called a creep in general. The secondary consolidation of soils proceeds with a time even if a stress state is fixed and thus is regarded to be a kind of the creep. The introduction of the creep due to the secondary consolidation into constitutive equations is of importance especially for the prediction of a deformation of soil structures for a long term after their constructions. It should be noted that an abrupt change of stress would not cause a plastic deformation since it takes a time for a slip of microstructure causing a plastic deformation to occur (there are no 'instant' inelastic strains, i.e. all inelastic strains require time to occur), while an elastic deformation occurs instantaneously. Therefore, it is thought that the stress goes out from the yield surface without producing a plastic deformation when it changes abruptly. The subloading surface model (Hashiguchi and Ueno, 1977, Hashiguchi, 1980, 1989, Hashiguchi et al., 1997) does not premise that the stress exists on the normal (conventional)-yield surface in a plastic loading process, introducing the subloading surface which passes always through the stress point even if the stress exists inside or outside the normal-yield surface and is similar to the normal-yield surface and letting the plastic modulus depend on the ratio of the size of the subloading surface to that of the normal-yield surface.

In this article the subloading surface model is extended so as to describe the elastoplastic and the creep deformation, taking account of the mechanical features mentioned above and formulating the novel loading criterion.

Symposium D1
Structural Dynamics, Nonlinear Dynamics and Control
Organizers
T.D. Burton & A. Barhorst
Texas Tech University, USA

Session: D1-1 Room: Auditorium **Time:** M10:00a-12:00p
Chairs: *T. D. Burton & A. A. Barhorst (Texas Tech)*

Numerically Stable Computation of the Lyapunov Characteristic Exponents for Continuous Dynamical Systems

Udwadia, F.E. and von Bremen, H.F.
University of Southern California, USA

A positive Lyapunov Characteristic Exponents (LCE's) of a nonlinear system is often used as an indicator of chaos. Methods for computing the LCE's in a numerically stable form have been presented when dealing with discrete dynamical system. However, for continuous dynamical systems the present methods can be so unstable that they actually fail to compute the LCE's for certain systems. This paper proposes a new method, which is numerically stable, for computing the LCE's of continuous dynamical systems. The general method is adapted to systems with small dimensions. The paper also presents the analytic expressions for the time evolution of the LCE's of a continuous two-dimensional constant coefficient dynamical system.

Analytical Criterion For Chaotic Dynamics In Flexible Spacecraft With Nonlinear Controller Damping And Nonautonomous Forcing

Gray, G.L.
Pennsylvania State University, USA, and
Mazzoleni, A.P.
Texas Christian University, USA

In this work, we study the attitude dynamics of a single body spacecraft that is perturbed by the motion of oscillating sub-bodies and a small flexible appendage constrained to undergo only torsional vibration. In particular, we are interested in the chaotic dynamics that can occur for certain sets of the physical parameter values of the spacecraft (*e.g.*, shape via moments of inertia, torsional natural frequencies, oscillation frequency of the sub-bodies, etc.) when energy dissipation acts to drive the body from minor to major axis spin. Energy dissipation, which is present in all spacecraft systems and is the mechanism which drives the minor to major axis transition, is implemented via a quantitative energy sink that is implemented using a nonlinear controller. This energy dissipation occurs whenever a spacecraft is not spinning about it principal mass moment of inertia axis and is an important driving force for chaotic dynamics in these systems. We obtain an analytical test for chaos in terms of satellite parameters using Melnikov's method. This analytical criterion provides a useful design tool for spacecraft engineers concerned with avoiding potentially problematic chaotic dynamics in their systems. In addition, we investigate the unique interaction that occurs between the driving frequency of the oscillating sub-bodies and the natural frequency of torsional vibration of the flexible appendage with regard to the onset of chaotic dynamics. This work is an extension of earlier work done by Gray *et al.*, in which they analytically investigated chaotic attitude dynamics occurring in simple spacecraft systems.

A Preliminary Study of the Application of Floquet Multipliers to Nonlinear System Identification

Zadoks, R.I.
University of Texas at El Paso, USA

The harmonic response of a three degree of freedom system is simulated numerically. This system is assumed to be fully coupled through the linear mass and stiffness terms, and it includes a single cubic nonlinear term ($g_1 = ay_1^3$) and a single harmonic excitation term ($f_1 = f\cos\Omega t$). After applying a coordinate transformation based on the linearized normal modes ($\{y(t)\} = [U]\{q(t)\}$), the resulting equations include complete sets of cubic nonlinear terms and harmonic excitation of every modal coordinate. For simplicity, linear modal damping is assumed. The Floquet multipliers (λ_i, i = 1,2,3,...,6), which are used to study the stability of the steady state periodic solutions, are traced as functions of the forcing amplitude f. The fact that the product of all of the Floquet multipliers for a system is essentially constant is used to determine forcing amplitude ranges where the inclusion of some of the nonlinear model coupling terms is important. Two examples are presented to highlight the insights gained from this study. Additionally, a method of using the Floquet multipliers to estimate the modal damping factors is presented.

Session: D1-2 Room: Auditorium **Time:** M1:30p-3:30p
Chair: *T.D. Burton & A.A. Barhorst (Texas Tech)*

A Helicopter Individual Blade Control with a "Smart" Spring at the Root

Solaiman, A. and Afagh, F.F.
Carleton University, Canada, and
Nitzsche, F.
National Research Council of Canada, Canada

Using the concept of Individual Blade Control (IBC), this work deals with the development and

simulation of a smart helicopter blade to tune the spectrum of loads associated with the non homogeneous forcing loads by superimposing a harmonic system on the rotating frame. The lumped parameter control approach is used in this investigation. The strategy is based on the concept introduced by Nitzsche, Lammering and Breitbach[1] in which the actuation to achieve aeroelastic stability is obtained by inducing torsional displacements at the root using a smart spring.

In order to accurately model the smart helicopter blade, one needs a realistic 3D dynamic model of an individual blade. Such non-linear equations of motion for the blade have been suggested by Hodges and Dowell [2]. Based on this work, a more simplified form of the blade equations of motion are used in the present study. These simplified equations that correspond to a more realistic representation of the real blade are valid for uniform, untwisted, cantilever rotor blades without chordwise offsets between the elastic, mass, tension and aerodynamic center axes.

The implementation of the smart springs in order to control the vibration of the helicopter blade is achieved by decomposing, K(q), the stiffness matrix of the system into three matrices, namely $K_a(q)$, containing the aerodynamic terms, $K_{so}(q)$, representing the constant blade structural and inertial properties, and $K_{st}(q)$ containing the variable blade structural properties. The controlling of the blade is achieved by manipulating the $K_{st}(q)$ matrix in the equations of motion.

1. Nitzsche, F., Lammering, R., Breitbach, E., "Can Smart Materials Modify Blade Root Boundary Conditions to Attenuate Helicopter Vibration?" in Fourth International Conference on Adaptive Structures, E.J. Breitbach, B.K. Wada and M. C. Natori editors, Technomic, Lancaster-Basel, 1994, pp. 139-150.
2. Hodges, D.H.; Dowell, E.H.; "Non-Linear Equations of Motion for the Elastic Bending and Torsion of Twisted Nonuniform Rotor Blades"; NASA TN D-7818; December 1974.

Dynamic Modeling and Experimental Verification of a Flexible-Follower Quick-Return Mechanism

King, S.A. and Barhorst, A.A.
Texas Tech University, USA

Presented here is the mathematical modeling and experimental verification of a flexible-follower quick-return mechanism. This mechanism is of special interest as the closed loop constraint manifests itself as a time varying load in the domain of the flexible member. The motivation for modeling this type of system is the current trend in the design of industrial equipment toward lighter weight more slender mechanism components used in order to achieve higher productivity and lower operating cost. As a result the usual rigid body assumptions made in the dynamic analysis of these systems are no longer valid. Flexibility of the machine elements must be considered in order to produce useful system models.

System equations of motion are generated using a hybrid parameter multiple body system modeling technique. The methodology allows rigorous formulations of the complete nonlinear, hybrid differential equations with boundary conditions, no lagrange multipliers are needed.

To verify the model an experimental mechanism was constructed and data was collected for several test runs with variations of the system parameters.

Modal Reduction of Some Non-Linear Finite Element Models Using High-Dimensional Invariant Manifolds

Pesheck, E. and Pierre, C.
University of Michigan, USA

The invariant manifold approach to the analysis of nonlinear systems has been shown to be an effective tool for the reduction of model size. This approach has been generalized such that a nonlinear model of arbitrary size may be reduced to a chosen subset of modal coordinates without eliminating the effects of the truncated modes. Algorithms have been developed which automate this procedure for nonlinearities of quadratic and cubic order in displacement. In addition, it is possible to include harmonic forcing in the invariant manifold, thus producing time-dependent manifolds and reduced equations with variable coefficients.

In order to apply these advances to engineering systems, it is necessary to work with Finite Element-based structural models. This study is concerned with the modal reduction of simple Finite Element models using the invariant manifold approach. Particularly, the investigation focuses on the accuracy of the reduced model as the number of retained coordinates is varied for several different systems. These include both forced and unforced, and internally resonant and non-internally resonant systems. In addition, results from both forced and unforced manifolds are compared. Appropriate conclusions are drawn regarding the utility of this approach in each case.

Effect of Internal Resonance on Model Reduction in Nonlinear Structural Dynamics

Burton, T.D. and Rhee, W.
Texas Tech University, USA

The problem considered is model reduction in undamped, unforced n-DOF structural dynamics models with cubic nonlinearities. The objective is to identify a subset of m<n "master" coordinates and to define a reduced dynamic model in which only the m master coordinates appear. The linear kernel of the

reduced model is to be exact (eigenstructure preserving), and the essential effects of the nonlinearities are to be preserved in the reduced model for small to moderate amplitudes. Two methods of model reduction are studied. The first is a simple "linear based" procedure in which the m lowest mode shapes of the linear kernel are used to define a linear coordinate transformation which enables one to eliminate the excess coordinates. This model provides the correct leading order frequency-amplitude behavior for periodic motions confined to individual modal manifolds. The second reduction method employs calculation of the nonlinear normal modes (as in Shaw and Pierre, *J. Sound Vib.*, **164**(1), 1993) as the means of model reduction. In this calculation the excess coordinates are expressed as polynomial series in the master coordinates and the master velocities, and the leading (cubic) terms in these dimensional manifold which is to represent the m lowest nonlinear modes. This "NNM based" reduction produces a reduced model which one would expect to be accurate to higher order than would the linear based reduction.

In applying the NNM based reduction to several simple spring mass systems of the type studied by Shaw and Pierre, we have found the accuracy of the reduced model simulation results to be affected significantly by the presence of internal resonances. Of course, the NNM based reduction beaks down if the parameters are exactly resonant, but significant inaccuracy also persists as the parameter values are moved reasonably far from their resonant values. The result is that the NNM based reduction is essentially invalid for a significant range of parameters. No such problems are encountered for the linear based reduction, for which the existence of internal resonance is not an issue. Results will be presented to illustrate these points.

Closed-form modeling of fluid-structure interaction - Navier-Stokes case

Ortiz, J.L.
Texas Tech University, USA

This work extends previous work by the author. A closed-form modeling of fluid-structure interaction problems is presented. Navier-Stokes equations are used to describe the fluid motion while Kane's method is used to model the dynamics of the interacting rigid multibody system. The fluid has a free surface and all inherent nonlinearities are taken into account. Therefore, no simplifications are made in handling sloshing effects, field equations and boundary conditions.

End result of this approach is a set of first-order differential equations for the motion of both the structure and the fluid. The numerical implementation is limited to the case of a rigid multibody system in which one body is a container carrying a sloshing fluid. Assembling the equations of motion involve solving a pressure equation for the fluid as a function of the accelerations of a moving frame attached to the rigid container. A discussion on the non well-posedness of the pressure equation in the fluid domain is addressed. Numerical examples are included.

Session: D1-3 Room: Auditorium **Time:** M4:00p-6:00p
Chair: *F. E. Udwadia (U. Southern California)*

Design of Adaptive Sliding Mode Controller for Robot Manipulators

Aledhaibi, A.M., Lu, B.H. and Huang, J-K.
Old Dominion University, USA

In this paper, a novel control scheme for accurate tracking control of robot manipulators is presented. The proposed scheme is to use the Variable structure systems for the control of manipulators. Variable structure systems (VSS) are a class of systems with discontinuous feedback control. The main feature of VSS is that it has the so-called sliding mode on the switching surface. Sliding mode control is a powerful approach for controlling nonlinear and uncertain systems. It is a robust control method and can be applied in the presence of model uncertainties and parameter disturbances, provided that the bounds of these uncertainties and disturbances are known. Hence, the theory of VSS can be used to design a variable structure controller (VSC) which induces the sliding mode and in which lie the robot arm's trajectories. Such design of variable structure controller does not require accurate dynamic modeling of manipulator; the bounds of the model parameters are sufficient to construct the controller. The proposed controller is applied to a two-link robot manipulator to show the applicability to the tracking control of MIMO systems. Computer simulation shows the robust performance of the proposed sliding mode control algorithm.

Time Delayed Control of Classically Damped and Non-Classically Damped Structural Systems

Udwadia, F.E., von Bremen, H.F. and Wilson, M.
University of Southern California, USA

The active control of structural systems modeled by linear matrix differential equations is presently an area of considerable interest. This paper deals with the time delayed control of general linear structural systems under the control of a large class of controllers. Results apply to classically damped systems as well as for non-classically damped systems.

The effect of time delay on collocated and non-collocated control of a linearly damped discrete structural system is examined. Conditions that assure the stability of general linear structural systems under the control of a large class of controllers is presented. For systems with a single actuator and using a large class of controllers (including PID type), it is shown

that there exists a range in the gain for which the system is stable regardless of the time delay (provided the open loop system is table).

The theoretical results are compared with experimental results conducted on a two-degree of freedom torsional system.

Sliding Mode Control-Dynamic Observer for a Slewing Flexible Link

Wilson, D.G., Parker, G.G., Starr, G.P. and Robinett, R.D.
University of New Mexico, USA

With the development of lightweight flexible structures comes structural flexibility. This will impact several application areas. Underground storage tank remediation, a Department of Energy application, requires slender manipulators to fit through small openings, yet once inside they must have a large workspace. The slender aspect ratio leads to structural bending orf the members and control of said structure suggests the need for vibration suppression. Future Space applications will require lightweight robotic arms capable of accurately positioning larger payloads and satisfying challenging slewing requirements. One way to reduce vibration is the development of advanced control strategies such as sliding mode controllers and dynamic observers for suppression of vibrations and enhanced slewing performance. In this paper we present a sliding mode controller and dynamic observer for a slewing flexible link. The approach is based on an output feedback sliding mode control algorithm. This algorithm is shown to be Lyaponuov stable. A dynamic observer is designed based on the flexible link dynamic equations. Only local stability can be shown for the dynamic observer. A dynamic simulation model was developed. Numerical simulations were performed to predict the performance of the combined controller-observer algorithm. The Sandia National Laboratories slewing flexible single-link experimental testbed was used to verify the algorithm performance. Results are shown for both numerical and experimental runs. The combined sliding mode controller-dynamic observer showed good tracking performance and minimal residual vibrations for the first two bending modes.

Vibration Control of an Elastic Shaft and Elastic Link Manipulator

Ankarali, A.A.
Seluk University, Trkiye, and
Mecitolu, Z. and Diken, H.
Stanbul Technical University, Trkiye

In robotics and other applications the members are designed to be rigid to satisfy the requirements, especially in robotics, to minimize the tracking errors. This design consideration results in heavy and slow manipulators which means high energy and time consumption. Designing lightweight manipulators that can carry heavy loads has been a popular research area recently. The usage of the lightweight and fast robots makes the control of the elastic manipulators important and a very difficult problem to overcome. The most important problem is the elimination of vibrations to enable the manipulator to follow the desired trajectory precisely with rather simple control methods.

In this study, the manipulator system is considered as a flexible Euler link attached to a flexible shaft which is driven by a servomotor. The manipulator is actuated by a cycloidal rise function. The system is analyzed in two steps as follows. In the first step the elastic shaft which transmits the motion from the servomotor to the elastic link is taken into consideration. The system is modeled as fixed-free rotating shaft at which free end carries an end rotary inertia. This inertia is included to model the mass moment of inertia effect of the link on the shaft axis. Later the equations of motions are solved again for the cycloidal rise function. Since the system is modeled as a continuous system, the disturbed rise motion applied to the link is obtained. In the second step the manipulator link that has a torsional spring at one end and free at the other is analyzed. In this case the new rise function which is cycloid plus contribution from the shaft elasticity is applied to this system. The new manipulator arm model and also the motion contains the effect of the shaft flexibility. The equations of motions are solved analytically and some simulation studies realized belonging to the tip point of the manipulator arm.

Since the inertial load acts only during the rise time tp, the vibration problem is transient. Mode summation techniques are used to find the solution.

Vibrational Method in Order to Value the Damage Caused by Unfit Lubrication of the Ball Bearings

Blosio, F.
Fiat Avio, Italy
Cavacece, M.
University of Cassino, Italy
Luvidi, C.
Fiat Avio, Italy

This paper presents the results of the vibration analysis performed on several rotating machines operating in presence of some faults. The vibration analysis has been used as diagnostic method in order to value the damage caused by unfit lubrication on the ball bearings of the machines. The prediction had a good correspondence with the practice.

Session: D1-4 Room: Auditorium **Time:** T9:30a-11:30a
Chair: *D. Segalman (Sandia)*

An Efficient, Hybrid Frequency-Time Domain Method for the Dynamics of Large-Scale Dry-Friction Damped Structural Systems

Guillen, J. and Pierre, C.
University of Michigan, USA

The steady-state response to periodic excitation of multi-degree of freedom structural systems with several attached dry friction dampers is studied. The general case of elastic/perfectly plastic dampers is considered. One distinguishing feature of the work is that no further approximation of Coulomb's friction law is made in the calculation of the friction force. Namely, the displacement of and the force transmitted by a friction damper are deduced in the time domain from the displacement and velocity of the corresponding degree of freedom to which the friction damper is attached. All other terms in the equations of motion are transformed, following a multi-harmonic balance procedure, into the frequency domain through the use of a Fast Fourier Transform. The resulting solution algorithm is thus hybrid in the frequency and time domains. The convergence of the method is ensured by a modified Broyden's algorithm, which is sued to solve iteratively the set of multi-harmonic nonlinear equations in the frequency domain.

The resulting solution procedure is robust and highly performant for all cases considered. It features fast convergence and yields extremely accurate results when compared to direct time integration, in part because no approximation of the friction force is made. For example, in the study, complete frequency responses are obtained for systems with 108 degrees of freedom and 36 dry friction dampers, over the entire range of friction parameters, and where as many as 17 temporal harmonics are taken into account. In the latter case the resulting 1836 frequency-domain equation, of which 612 are nonlinear, are handled effortlessly by the Broyden solver.

The method can handle both friction dampers that are attached to ground and the general case of dampers that connect two degrees of freedom of the structure. As an application, a cyclic assembly of beams coupled by linear elastic elements is studied, with friction dampers located between the beams and the ground or between two beams, or both. This system is a simplified model of a dry-friction damped bladed disk used in turbomachinery applications. Assemblies with various number of beams (blades) and of friction dampers are considered. Results are obtained for both tuned and mistuned configurations of these systems subject to various traveling wave "engine order" excitations, for a variety of structural and friction parameters. Interesting, complex features of the nonlinear response are revealed, such as: motions for several stick-slip phases per period; localized motions for mistuned systems, which feature mostly sticking motion at most blades and mostly slipping motion at a few blades; subresonances; effects of higher harmonics.

This work is believed to be the first to develop a robust solution procedure for predicting the complex, multi-harmonic response to periodic excitation of large-scale structural systems with many friction dampers. Current efforts include the extension of the method to study the stability of autonomous, dry-friction damped, multi-degree of freedom systems with negative viscous damping. Preliminary results for the latter topic will be presented.

Modeling, Simulation and Verification of Contact/Impact Dynamics in Flexible Articulated Structures

Hariharesan, S. and Barhorst, A.A.
Texas Tech University, USA

The minimum set of non-linear hybrid differential equations that models the dynamics of flexible structures undergoing contact/impact is developed using a hybrid parameter multiple body (HPMB) methodology. The complete motion regime i.e., pre-contact/impact free motion, contact/impact and post-contact/impact constrained motion, is modeled. The model includes the dynamics due to interconnecting rigid bodies, the driving motors and gearboxes and backlash in the gearbox. Also, Coulomb friction in the constrained motion regime is included in the model. The above model is experimentally verified through a two-flexible link manipulator that undergoes the complete motion regime mentioned above.

Minimal Modeling of Multi-Point Contact with Friction in Multiple Rigid

Nugent, A.L. and Barhorst, A.A.
Texas Tech University, USA

Presented here is the minimal mathematical modeling of multi-point contact with friction in a planar multiple rigid body system. System equations of motion are generated using Kane's form of the Gibbs-Appell equations. Pseudo-velocities are used to determine the non-active forces, which results in the determination of the friction forces, during manipulation of an object. The rigid body system consists of a planar finger-thumb combination performing the manipulation of a cylinder on the last link of each digit. The mathematical model predicts when the conditions exist for the cylinder to roll, slip, or stick. The state space of the model is of variable structure, but the switching between structures is simply determined.

Previous research has shown that friction forces during manipulation can be calculated using the linear

complementarity problem (LCP) and the penalty/augmented Lagrange multiplier method. The LCP formulation and the Lagrange multiplier method add extra complication to the problem at hand and solution convergence is not guaranteed. In this paper we intend to show that the use of pseudo-velocities for the determination of friction forces avoids the complexities and pitfalls of the previously mentioned methods.

Control of Mechanical System with Nonholonomic Constraints

Larin, V.B.
Institute of Mechanics of National Academy of Sciences of Ukraine, Ukraine

Nonlinear algorithms of stabilization of program modes of movement of controlled wheel system are presented. The problem of control of vehicles is considered in kinematic and in dynamic statements.

A problem of control of systems with nonholonomic constraints takes an important place in development of transport robots (see, for example, [1-3], where are the further references). In the present paper a problem of stabilization of movement of system with nonholonomic constraints is considered with reference to the wheel's model. In the kinematic approach problems of stabilization of two types of program movements are examined: rectilinear movements and movements on a circle. Choice of these program modes is motivated by the following reason. In the first, these modes of movements are realized at the elementary laws of a control (fixed position of a steering wheel), secondly, an initial trajectory of movement of robot frequently can be approximated by rather small number of arches and segments. At the decision of a problem of stabilization, deviation from these program movements it is not assumed small, i.e., it is created the nonlinear algorithms of stabilization.

In the kinematic approach, the procedure of synthesis of algorithm of stabilization is considered in statements when control influence is an angular velocity of turn of a steering wheel. Further this problem of synthesis is considered with reference to the dynamic model (Lineykin's model [4]). This model is derived at the assumptions similar to accepted in [3] (is not taking into consideration the energy of rotation of wheels, is away sliding etc.). It is shown, that problem of synthesis of the algorithm of stabilization for this model in dynamic statement is reduced on mentioned above kinematic problem and a problem of stabilization of speed of apparatus. It is marked, that in many problems it is possible to exclude, procedure (mentioned above) of approximation of initial trajectory by segments and arches. With this purpose, the algorithm of stabilization is generalized on the case of tracking of a given trajectory.

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Session: D1-5 Room: Auditorium **Time:** T1:00p-3:00p
Chair: *R. Zadoks (Texas at El Paso)*

Stability Analysis of Diamond Turning Manufacturing Processes

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University of Maryland, USA

To lower manufacturing costs by increasing material removal rates leads to highly dynamic manufacturing processes. In order to also meet tolerance requirements the internal nonlinearities arising from the cutting mechanics must be taken into account. Diamond turning in ultra-precision machining is a cutting process that produces superior surface finish that is characterized by depths of cut ranging from 20μm for roughing cuts to 1 μm or smaller for finish cuts. A typical tool used for diamond turning is a round nosed tool with a tool tip radius of 500 μm. Regenerative machine tool vibration (chatter) is an important mode of instability in turning processes. Traditionally turning processes have been modeled using an orthogonal cutting model. In that model the tool is assumed to be a wedge that is much wider in the direction perpendicular to the cutting direction than the material being removed and a large ratio of chip width to uncut chip thickness. The forcing function in the orthogonal cutting case is proportional to the workpiece's specific cutting energy and chip area. The chip area is usually assumed to be proportional to be a function of the chip thickness variation, which is expressed as the difference of the delayed tool edge position and the resent position where the delay is the time period of one revolution. However, in the case of diamond turning with a round nose tool the chip area is determined as a function of the tool radius, the feed rate as well as the current and past position of the tool in the workpiece, but not as the difference of these two

positions. In fact it is a highly nonlinear function of these quantities. In both orthogonal and round nosed tool cutting the corresponding mathematical models involve retarded (delay) differential equations. The characteristic equations for both models are transcendental functions with an infinite number of eigenvalues. As long as the parameter representing the ratio of the feed rate to chip width in round nosed tool cutting is small one can show that the coefficients involved with the characteristic function for round nosed tool cutting are small perturbations of the coefficients for the orthogonal cutting characteristic equation. Implicitly then the infinite number of frequencies that compose the critical eigenvalues for the round nosed tool model are small perturbations of the frequencies for the orthogonal cutting model. The perturbation series terms can then be computed in such a way that the techniques used in orthogonal cutting to generate the stability lobe boundaries can be adapted to the round nosed tool case. Once the stability boundaries are found in the round nosed case the techniques used by some researchers to demonstrate the Hopf bifurcation at the stability boundaries for orthogonal cutting can be modified to demonstrate Hopf bifurcation in the round nosed tool case. Multi-scale expansion methods and projections onto center manifolds coupled with normal form theory are extendable as long as care is taken in processing the perturbation terms.

Suppression of Regenerative Chatter via Impedance Modulation

Segalman, D.J. and Butcher, E.A.
Sandia National Laboratories, USA

A new technique for the suppression of machine tool chatter in turning based on modulation of the system impedance is analyzed. The impedance modulation technique suggested by Segalman and Redmond [1] is shown to be effective in scrambling the lag signal which could otherwise cause unbounded regenerative vibration in the milling process. The method examined here involves modulating the machine tool stiffness at a frequency twice that of the turning rate. The governing equation is a time-periodic differential delay equation which is examined for stability using the method of harmonic balance to obtain a characteristic equation and subsequent numerical root-finding techniques to obtain the stability boundary. Process damping is not included. The results are verified using the Nyquist stability criterion since the transcendental equation contains an infinite number of roots. It is found that the use of two harmonics is sufficient to give accurate results, which were plotted in the form of familiar stability diagrams in the two-parameter plane of turning frequency and cutting depth. It is found that the modulated unstable lobes lift up with a decrease in the frequency similar to process damping effects. The lift reaches a maxi mum and then decreases again while the unstable lobes become `out of phase' with the unmodulated ones. The region of maximum lift is found to move to higher frequencies with an accompanying increase in the modulation amplitude while the amount of maximum lift as well as the maximum interval width of stable frequencies for a given cutting depth also increases. It is shown in this way that the impedance modulation technique successfully scrambles the regenerative process that leads to chatter and widens the stability region. For the modulation amplitudes considered here, however, the parametric impedance modulation most significantly augments the stable region within the low speed regime while leaving the unstable lobes at higher frequencies much the same. The change in stability of the response for four parameter sets are examined as a function of increasing modulation amplitude by using the stability diagrams as well as Nyquist plots and growth exponents computed from transient simulations of the vibratory response.

[1] Segalman, D. J. and J. Redmond, `Chatter suppression through variable impedance and smart fluids', published in proceedings of the 1996 SPIE Symposium on Smart Structures and Materials, Commercial Applications of Smart Structures Technologies, SPIE Proc. Vol. 2721, edited by C. Robert Crowe.

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Optimum Excitation System Mass - Efficiency Design of the D. C. Compound Motor

Kowalski, J., Corrales, J. and Pedronio, P.
University of Bío-Bío, Chile

The objective of the paper is to describe the method for selecting optimum design features of the D. C. compound motor with a given structure for minimum excitation system mass and maximum efficiency by fulfilling all constraints. The optimization problem is reduced to finding the minimum of the modified additive dimensionless scales function including linear power loss index [1] in a 12 - dimensional space bounded by 29 or 30 operation and design inequality constraints based on Kuhlmann´s theory [2]. To increase the efficiency of motor modeling, on use the first author's idea of two - level hierarchic optimization modeling system [3]. As an application example, an American existing motor has been optimized. The polyoptimization problem has been solved for a discrete net of scales factors, and the polyoptimum preferred design has been selected. Praxiological analysis of the solution [4] has been carried out. Technical and economical advantages proceeding from the solution achieved are shown.

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2. Kulmann, J.H., Design of Electrical Apparatus, Wiley, New York, 1983.
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Session: D1-6 Room: Auditorium **Time:** T3:30p-5:30p
Chair: *D. Gilsinn (NIST)*

A New Computational Method in Nonlinear Oscillatory Analysis

Singh, M.
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Dai, L.
Red Deer College, Canada

This paper is devoted to the development of a novel numerical method for the solutions of nonlinear oscillatory problems which are common in engineering dynamics. Based on a piecewise-constant technique [1] and Taylor series expansion, the original information including in the governing equations of the oscillatory systems are mostly transferred into the numerical solutions.

In solving the differential equations of nonlinear oscillatory systems by the existing numerical methods such as Euler's method, Taylor-series method and Range-Kutta method [2], conventionally, the differential equations are transformed into a system of first-order differential equations. On the basis of the first-order differential equations, a recurrence relation for numerical calculation is then developed. The numerical solution so produced can only be discrete. With the introduction of a piecewise constant argument $[Nt]/N$ and Taylor series expansion, the numerical solutions are so developed in this work that a linear oscillatory system is established between the two points $[Nt]/N$ and $([Nt]+1)/N$. Therefore, unlike the discrete solutions produced by the existing numerical methods, the numerical solutions produced by the present method are continuous everywhere on the entire time range considered. In numerically solving the oscillatory problems by the present method, the form of the corresponding original differential equations remains mostly unchanged. Therefore, the solutions derived by the present method are very accurate with good convergence in comparing with the existing traditional methods.

The present method can be easily used in solving the retarded and advanced functional differential equations with $[t]$ or $(t \neq n[t])$ as the piecewise constant arguments [3]. An investigation of the dynamic behavior of a highly nonlinear driven Froude pendulum is carried out by making use of the present method. Periodic, quasiperiodic and chaotic motions of the pendulum are investigated with varying system parameters and different initial conditions.

1. Dai, L. and Singh, M.C., "An Analytical and Numerical Method for Solving Linear and Nonlinear Vibration Problems," International Journal of Solids and Structures, Vol. 34, pp. 2709-2731, 1997.
2. Gerald, C.F. and Wheatley, P.O., Applied Numerical Analysis, Addison-Wesley Publishing Company, New York, 1989.
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On Computing the Largest *p* LCE's of Discrete Dynamical Systems

von Bremen, H.F., Udwadia, F.E. and
Proskurowski, W.
University of Southern California, USA

The computation of the Lyapunov Characteristic Exponents (LCE's) is important because the exponents help characterize the behavior of dynamical systems. If one is interested in determining whether a dynamical system is chaotic or not, often just a few of the largest LCE's may provide the answer.

In this paper two efficient and numerically stable methods to determine the largest p Lyapunov characteristic exponents of discrete dynamical systems are presented. The two methods are based on the HQRB method which is an adaptation of the Householder QR transformation method. The two methods presented are numerically backward stable since they are based on Householder transformations. The methods are compared with the commonly used classical Gram-Schmidt method on the basis of computational efficiency.

Design of Adaptive Fuzzy Sliding Mode Control for Robot Manipulators

Aledhaibi, A.M., Abdel-Motagely, K.A. and
Huang, J-K.
Old Dominion University, USA

In this paper, new control scheme for accurate tracking control of robot manipulators is presented. The proposed scheme combines the fuzzy logic control with the sliding mode control. Fuzzy logic controllers have been applied successfully in many applications and were shown to be superior to the classical controllers for some nonlinear systems. Sliding mode

control is a powerful approach for controlling nonlinear and uncertain systems. It is a robust control method and can be applied in the presence of model uncertainties and parameter disturbances, provided that the bounds of these uncertainties and disturbances are known. This principle provides quidance to design a fuzzy logic controller for system stability. Therefore, a control scheme called sliding mode-based fuzzy logic control is proposed, in which the principles of fuzzy logic control and sliding mode control are combined. The main disadvantage of fuzzy logic controllers is the generation of the control rules. This problem can be solved by using the self-organizing fuzzy logic controller which is capable of generating and modifying control rules based on an evaluation of the system performance. The modification of the control rules is derived from the system phase plane and by using the sliding mode control. The proposed controller is applied to a two-link robot manipulator to show the applicability to the tracking control of MIMO systems. Computer simulation shows the robust performance of the proposed sliding mode self-organizing fuzzy logic control algorithm.

A General Theory of Flotation

Ortiz, J.L.
Texas Tech University, USA

A general closed-form approach for coupling the motion of a floating multibody system is addressed. The approach is based on a general methodology for handling fluid-structure interaction problems presented earlier by the author. Derivations are presented for the case of a rigid multibody system in which only one body is floating. The case of multiple of a multibody system with two or more floating bodies can be handled similarly. The fluid is modeled using potential flow theory and Rayleigh damping was chosen to model dissipative effects.

The approach is closed-form in nature and no simplifications are made in field equations and boundary conditions. Numerical examples are presented.

Acquisition and Tracking with Higher-Order Plant and Nonlinear Regulation of Bode Diagram

Lurie, P.J., Ahmed, A. and Hadaegh, F.Y.
California Institute of Technology, USA

Acquisition and tracking systems are designed to operate in two modes: acquisition mode when the error is large, and tracking mode when the error is small. An example of the acquisition/tracking type is a pointing control system for a spacecraft-mounted camera, in which a rapid retargeting maneuver is followed by a slow precise scanning pattern to form a mosaic image. When the error signal is large, i.e. the system is in the acquisition regime, the controller should respond as rapidly as possible, i.e. the feedback bandwidth should be wide, limited by the plant structural modes. In the acquisition mode it is not necessary however that the feedback be very large, since the error is big anyway. In contrast, in the tracking regime, the feedback bandwidth needs to be reduced to reduce the output effects of the sensor noise, but the value of the feedback should be made rather large to minimize the tracking error.

The typical object of control is high-order, with flexible modes, and needs to be controlled closed-loop in robust and optimal way. The controller should provide optimality of the system performance in both modes of operation and optimal transition between the modes of the operation. The controller must be, therefore, high-order and nonlinear.

While for acquisition and for tracking, separately, a controller with close to optimal behavior can be found even for flexible plants, a smooth transition between them presents a serious challenge. The controller is high-order, and all intermediate responses also must be high-order. Finding and implementing these responses, and then switching between them without creating excessive transients presents formidable difficulties.

In this paper we describe a design of a controller with high-order linear part and a single nonlinear non-dynamic link, to obtain smooth regulation between the limit conditions. Bode theory of symmetrical regulators is utilized but with a nonlinear link replacing the variable linear link. Provisions have been made to guarantee minimum phase of the regulator during the transitions and close to optimum transient responses.

Acknowledgment. The research was carried out by the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautic and Space Administration.

Symposium D2
Control Opportunities in Materials Processing
Organizer
J. Berg
Texas Tech University, USA

Session: D2-1 Room: CUB B1-5 **Time:** T3:30p-5:30p
Chairs: *T. D. Papathanasiou (U. South Carolina)*
X. Ren (Utah State)

Modeling Fine-Scale Structures by Integro-Differential Equations

Ren, X.
Utah State University, USA

Martensite transformations are phase transformations that produce a change of shape and a change of crystal symmetry. Shape-memory materials are materials that are extremely malleable in the martensite phase below a transformation temperature, but that return to a 'remembered' original shape when heated above the transformation temperature. Coherent phase transitions of crystalline solids lead to mixtures of distinct phases or phase variants with characteristic fine-scale structures. A nonlocal theory involving integro-differential evolutionary equations is proposed to answer the questions of determining the characteristic scales, and modeling the generation and the propagation of the microstructures. This theory lies between the traditional microscopic quantum theory which uses Schodinger's equation and the macroscopic elasticity theory which uses elliptic and hyperbolic partial differential equations. Periodic solutions are found to match oscillatory phase patterns. "Generalized" traveling solutions which describe the formation of the oscillatory patterns out of uniform patterns are also studied.

Meso-Scale Modeling in Composite Materials using the Boundary Element Method

Papathanasiou, T.D
University of South Carolina, USA

Prediction of the effective properties of composite materials from detailed knowledge of their microstructure is an important issue in materials science and engineering. This is not surprising, since the better use of novel materials with unique property profiles (such as gradient composites or enhanced-flow preforms) as well as the application of the concepts of "intelligent" or "product-oriented" processing hinge on exactly this capability. Interest in this direction has been continuous and strong for decades, but detailed computational investigation of microstructural factors has been hindered by the requirements of 'domain methods' (finite elements, finite differences) in terms of meshing and computational resources. Contrary to domain methods, the Boundary Element Method (BEM) requires meshing only of the boundaries of the domain of interest. In complex multiply-connected microstructures this is a decisive advantage. This talk will present results of the application of the BEM to problems related to the prediction of the effective properties of composite materials based on detailed microstructural information, namely:
(i) a study of the effect of configurational factors on the stiffness of short-fibre-reinforced composites and
(ii) a computational analysis of flow across perturbed arrays of fibers and across arrays of fiber tows.

In the context of the former, we investigate the range of validity of the Halpin-Tsai equation and of its variants by carrying out numerical experiments in composite samples which contain up to 200 individual short fibers, randomly dispersed in an elastic container. In the context of the latter, we study the effect of structural imperfections on the effective permeability of arrays of unidirectional fibers and also investigate the influence of fiber clustering on permeability. Models for the permeability of assemblies of fiber tows are proposed based on these numerical results.

Hydraulic Permeability of Fibrous Media Revisited

Clague, D.S.
Los Alamos National Laboratory, USA

The purpose of this study is two fold. First, we would like to demonstrate that the Lattice Boltzmann simulation method is a viable tool for the study of complex media. Second, we will employ the Lattice Boltzmann simulation method to explore ordered and disordered fibrous media. Simulation results are compared with known and accepted results for ordered and disordered media. The simulation results exhibit excellent agreement with these existing theory and alternative simulation methods for the entire range of possible fiber volume fractions. The observed macroscopic behavior, hydraulic permeability, shows a distinct connection with the details of the flow field. This connection is explored and elucidated for ordered and disordered fibrous media for both unbounded and bounded flows at vanishingly small Reynolds numbers.

Microstructural Modeling of the Evolution of Stress and Plastic Strain Fields During Fabrication Cool-Down of Fiber Reinforced IMC's

Baxter, S.C.
University of South Carolina, USA , and
Pindera, M-J.,
University of Virginia, USA

Residual stresses which develop during the cool down phase of composite fabrication can be high enough to degrade properties prior to service. Sufficiently large stresses can prematurely damage the composite, resulting in microstructural damage such as transverse fiber cracks, matrix cracking or filament breaks within a fiber tow. Using a microstructural description of the material system it is possible to track the evolution of local stresses and plastic strains for possible contributions to failure modes, in order to assess the effects of this phase of fabrication more accurately.

The generalized method of cells micromechanics model, GMC is used to characterize the microstructure of a continuously reinforced intermetallic compound, known as APA/IC-50, (Al_2O_3 / Ni_3Al). This material system consists of a nickel aluminide matrix, (IC-50), continuously reinforced by an aluminum oxide hybrid fiber. The fiber, developed by Cantonwine[2] is made from a tow of aluminum-oxide filament infiltrated with porous aluminum-oxide. It is known as the A-PA fiber, for Alumina Porous Alumina. GMC, which allows a detailed geometric description of multiphase materials, was used to develop effective properties of the hybrid fiber, including properties of the porous binder, as well as the fiber/matrix system.

GMC's microstructural characterization is embedded in two continuum scale models of the cool-down phase of composite fabrication. The continuum models correspond to 1.) a baseline model of idealized processing conditions, (unconstrained), and 2.) an extension to the process model which includes a tooling constraint generally associated with fabrication techniques such as hot isostatic pressing, vacuum hot pressing or die casting, (constrained). It is shown that residual stresses, at the end of the process, differ very little with either continuum model. The stresses that evolve during the cool-down, however, are significantly different for the two models. In the unconstrained model the driving mechanism for the developing stresses and plastic strains due to thermal cool-down is the mismatch between the coefficients of thermal expansion of the fiber and matrix materials. In the constrained model this effect becomes secondary to the mismatch between the thermal expansion coefficients of the composite and the constraining can. In the constrained model, in-plane tensile stresses develop which are large enough to produce microstructural damage in the form of transverse fiber cracks, matrix cracking or filament breaks within the fiber tow.

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Applications of Magnetic Resonance Imaging (MRI) In Process Engineering: Porous Media

Mantle, M.D. and Gladden, F.L.
University of Cambridge, United Kingdom

The ability of magnetic resonance imaging and spectroscopy to provide non-invasively, spatial and chemical information is well established in medical fields. However, these techniques have only recently been exploited in the area of process engineering. This presentation aims to show how our laboratory has been using MRI to provide structural, dynamical and chemical information on porous materials. The talk covers three main areas:

(1) Structure-flow correlations in Packed Beds.
(2) Remediation Studies using MRI
(3) Localised Velocimetry studies in ordered fibrous media.

Packed columns are of considerable interest from both industrial and academic viewpoints. Many industrial processes such as catalytic cracking and hydrogenation reactions involve multiphasic flow over a column or reactor packed with some kind of catalyst. Work done in our laboratory has addressed some of the related problems on a more fundamental level. Here we have used 3-dimensional MRI and MRI velocimetry to characterise the pore space and velocity fields in a glass bead/water pack. These studies have been extended to examine two phase liquid systems in porous media. In particular the dissolution and/or mobilisation of one phase by the other has been investigated. Such information is of considerable value in models of soil remediation. These studies have shown the importance of pore scale velocity heterogeneity in the dissolution. Experimental and computational results are also presented for flow through fibrous porous media. Here the system comprises a network of cylindrical fibers (bundles) separated by spaces through which fluid may flow. Similar systems can be found in many engineering applications such as liquid composite moulding, filtration, flow in hollow membrane bioreactors and heat transfer in connective heat exchangers. We have studied experimentally using MRI and computationally using the boundary element method (BEM) the distribution of velocities within cylinder arrays and a narrow gap placed between the arrays and the wall in a

Hele-Shaw cell. Model predictions are in good agreement with MRI measurements

Session: D2-2 Room: Auditorium **Time:** W9:30a-11:30a
Chair: *R. P. Bray (Texas Instruments)*

Optimal Design and Control Problems in the Manufacturing of Advanced Nanoscale Layered Materials

Burns, J.A.
Virginia Polytechnic Institute & State University, USA

In this presentation we discuss several optimal design and feedback control problems that arise in the control and optimization of nanoscale materials manufacturing.

We motivate the talk by describing a specific reactor design problem and use this problem to motivate the theoretical and computational issues. We present a computational algorithm based on the Sensitivity Equation Method (SEM) and indicate how efficient computation of state sensitivities can be exploited to optimize reactor design and to identify which parameters are most effective for active control.

The development of practical feedback controllers for enhanced manufacturing is one of the most challenging problems in this area. Two important difficulties are:

i) the optimal location of sensor/actuator pairs
and
ii) the construction of a low-order observer needed to estimate those states that can not be sensed.

In the design of low order controllers for such complex dynamical systems, it is common practice to first construct a reduced order open-loop model and then use this reduced order lumped parameter model in the controller design. Although this approximate-then-design method often works well, it is well known that this approach can lead to erroneous results and one must exercise care to ensure that the resulting design is robust.

We shall describe a distributed parameter approach to feedback control and indicate how this approach might be used to address some of the problems that arise in manufacturing nanoscale materials. In particular, we illustrate how distributed parameter control theory can be combined with computational mathematics to provide a practical approach to optimal sensor location and controller reduction. We give examples where this design methodology has been applied to control problems involving thermal processes and fluid flows.

Finally, we close with a discussion of mathematical and computational issues that need to be addressed before the method can be extended to more complex manufacturing processes.

Modular Feedback Design in Epitaxial Processes

Warnick, S.C. and Dahleh, M.A.
Massachusetts Institute of Technology, USA

Industry increasingly demands flexible solutions to their engineering problems to remain competitive in an uncertain, dynamic environment. Modular solutions satisfy these demands by recycling existing technology in the realization of new solutions.

In a feedback context, this implies that the controller should decompose into subsystems associated with each of the subsystems forming the "plant." Thus, as various improvements are made on different technological aspects of the plant, only the subsystems of the controller associated with these parts need to be redesigned; the entire controller should not need to be redesigned from scratch.

The trade-offs with such an approach depend on whether the objective function governing performance tractably decomposes in a manner consistent with the structural decomposition of the plant. In general, we might expect that a modular design could seriously degrade performance.

This work explores the feasibility of modular feedback designs for the control of Metalorganic Chemical Vapor Deposition (MOCVD) and Gas-Source Molecular Beam Epitaxy (GSMBE), using ellipsometry as an *in-situ* sensor technology. In particular, it is first shown that the dynamics of these processes, and their relationship to each other, encourage a modular approach to controller design. Next, previous work is reviewed that experimentally demonstrates the use of ellipsometry for feedback in a modular context. Finally, a control-oriented model of ellipsometry is developed and analyzed in terms of its effect on the control problem. The resulting impact on modularity in the feedback design is then discussed.

The VMBE System: Virtual Prototyping Within Reach

Meyer, D.M., Tucker, M. K., Bennett, A.D. and Engelmann, A.P.
University of Colorado, USA

We describe the VMBE --- Virtual Molecular Beam Epitaxy --- system. This is a simulation written in MATLAB/SIMULINK that successfully captures highly nonlinear dynamics of III-V compound semiconductor epitaxial growth by molecular beam epitaxy (MBE). In advanced semiconductor growth, crucial experiments are costly and time consuming. A virtual experimental platform in this area is a natural and important development. Moreover, VMBE provides a platform for designing and testing advanced control methods designed to increase the run to run and batch to batch repeatability and accuracy of the MBE process. For example, effusion cell control algorithms, such as proportional-integral-derivative (PID), nested

PID, and nonlinear control methods have been designed and tested using the VMBE system. VMBE shows how the different compensators work under a variety of real-life work conditions (i.e. varying operating points and melt levels). We present examples of all these simulations and insights into what control methods appear promising. Internally, the VMBE system has three main dynamic models, all appropriately coupled. There is an effusion cell model, a substrate thermal model, and an epitaxial growth model. VMBE thus tracks *all* the important dynamic parameters in a real III-V growth by MBE. Each model is, mathematically, a set of nonlinear driven ordinary differential equations. Parameters in the models have been ``tuned" from actual data, and we present analysis and results of system identification. VMBE predicts several interesting effects, some of them previously known (e.g. flux transients) and others not as widely recognized (e.g. Indium rich initial layers in the growth of InGaAs). True virtual prototyping with VMBE is within reach.

Application of Generic Modeling to Plasma Etching Systems

Bray, R.P
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Rhinehart, R.R.
Oklahoma State University, USA

In the semiconductor industry, process modeling has become an effective tool in reducing the cost of the development of new integrated circuits. Among the many processes involved in fabricating an integrated circuit, plasma or dry etching is the most common method of selectively removing material from a surface in order to transfer a pattern. Rigorous modeling of both the bulk plasma phase physics and the substrate surface reaction chemistry in order to predict etch rates is a difficult and time-consuming task, however. Simplified approaches are therefore required to keep the modeling problem tractable.

The typical simplified approach in industry is response surface modeling (RSM). RSM relates the modeled phenomenon directly to process variables such as pressure or power setting through an empirical polynomial. While RSM provides a relatively fast way of arriving at a model, empirical polynomials have weak predictive properties outside the range of fitted data and offer little physical understanding of the system. RSM also relies heavily on constant, ad hoc experimentation, which can be expensive.

An alternative approach is term "generic modeling." Generic modeling groups surface reactions according to type and permits the derivation of an etch rate expression for a given type of reaction, rather than for a particular system. Guiding the derivation is a set of reasonable, generally applicable simplifying assumptions about the physics and chemistry involved. In this approach, the etch rate is related to physical quantities such as ion fluxes and neutral etchant concentrations, approximated by direct measurement, rather than process variables. The result is an expression that, although derived once, has the potential to apply to multiple etching systems without modification. As in RSM, the parameters of a generic model are regressed from data. But the generic model usually has fewer parameters for regression than the corresponding RSM. Because it is a simplified representation of physical phenomena, the generic model permits a greater confidence in predicting etch rates outside the range of fitted data as well as yielding an understanding that can be incorporated in the user's knowledge base.

The generic modeling method will be demonstrated on experimental data for chlorine plasma etching of polysilicon; tetrafluoromethane/oxygen plasma etching of polysilicon and silicon dioxide; and oxygen plasma etching of photoresist. A method of model validation employing nonparametric statistics will also be presented.

Session: D2-3 Room: Auditorium **Time:** W1:00p-3:00p
Chair: *C. Doumanidis (Tufts U.)*

Verification of Bond Quality Improvement for Closed Loop Temperature Control of the In-Situ Thermoplastic Composite Tape-Laying Process

Sun, W.C., Mantell, S.C. and Stelson, K.A.
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In thermoplastic tape-laying, the temperature at the interface between the top ply and substrate is critical to achieving interlaminar bonding. In previous work, a three-lump process model was developed to represent the process dynamics. Based on this process model, a Kalman filter and state feedback controller were built to successfully predict and control the interlaminar bonding temperature during the process. A practical advantage of this controller is that the only measurement required is that of the heater temperature.

In this work, two methods are used to examine the bond quality when applying the previously developed control method. One is a microscopy study and the other is a lap shear strength test. The microscopy pictures show the interlaminar bond width is reduced as the bonding temperature is increased. The lap shear tests show the bond strength is significantly improved as the bonding temperature is raised. Both test results have consistently demonstrated the strong causal relationship between interlaminar bonding temperature and bond quality. The results show that the previously developed control method can produce high quality laminates by using temperature feedback. In the future, a non-destructive sensing method will be implemented for feedback and real-time monitoring of bond quality during the process.

Extrusion Process Control: Modeling, Identification, and Control

Tibbetts, B. and Wen, J.T.
Rensselaer Polytechnic Institute, USA

This paper develops a methodology for process control of bulk deformation - specifically, extrusion. We discuss the process model development, parameter identification, and control, including both off-line optimization and on-line press load and/or extrudate temperature feedback.

We have developed a novel process model based on the upperbound method based approximation of the deformation field and the heat diffusion equation model for the temperature distribution. In the axisymmetric 2D case, the temperature model (diffusion equation with heat contribution from conduction, advection, deformation, and friction both with the container wall and in the shear zone) is discretized using spectral approximation. Since the nonlinear terms in the model can all be computed off-line and stored in the tabulated form, process simulation can be executed in near real time

Several key process parameters, coefficients of friction for metal/container interface and metal/dead-metal-zone interface, and boundary heat transfer coefficients, enter into the heat equation linearly. We show that they can be estimated through temperature and load measurements using the standard least-square method. The form of the ram velocity profile is also shown to affect the parameter identifiability significantly.

The process model can be used to optimize for the initial billet temperature profile and the ram velocity profile. Constraints on the maximum strain rate can also be incorporated. If the extrudate temperature and the press load are available for on-line feedback, we show that the extrudate temperature can be regulated around a set point. However, the nonlinear flow stress (dependence on both the strain rate and temperature) does pose a challenge to the control analysis.

To illustrate the overall approach, an example with plant trial data is provided.

Parameter Sensitivity and Robust Feedback Controllers for Consolidation Processing of Titanium Matrix Composites

Vancheeswaran, R. and Wadley, H.N.G.
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Meyer, D.G. and Piatt, T.
University of Colorado, USA , and
Kosut, R. L.
SC Solutions Inc., USA

The successful consolidation of fiber reinforced titanium matrix composite monotapes is dependent on the elimination matrix porosity while simultaneously minimizing fiber microbending/fracture and the growth of reaction products at the fiber-matrix interface. In previous work, model predictive planning concepts (R. Vancheeswaran et al., Acta Mater., 45(10), 1997, pp.4001-4018), were combined with dynamic consolidation models (R. Vancheeswaran et al., Acta Mater., 44(6), 1996, pp. 2175-2199), to develop a method for finding near optimal process schedules which result in composites of acceptable mechanical performance. The performance of these process schedules were dependent on the set of deterministic (nominal) material and geometric parameters. Unfortunately in the real world, these key model parameters are subject to some variability. This presentation will first evaluate the extent to which the variability in the geometric and material parameters affects the key final microstructural attributes of the composite (which determine its mechanical performance). The effect of the variability is found to be drastic and thus cannot be ignored in real processing. A parameter sensitivity analysis is then performed to understand how the variability in each parameter affects the final microstructure of the consolidation process. A model predictive controller (MPC) is then used in conjunction with microstructure attribute sensors for density and fiber fracture to drive the microstructure of a plant with uncertain material properties to a desired goal state. The process schedules of the MPC controller are then compared with other feedback control designs for the robust regulation of consolidation. The efficacy of the methods and the designs are illustrated by exploring the design of process schedules for the Ti-6Al-4V/SCS-6 titanium matrix composite with variability in the matrix properties. The model predictive controller shows good robustness and produces process schedules that give acceptable results over a range of parameter variation. These controllers would increase the high-yield manufacture of titanium matrix composites.

Thermal Control of Materials Processing In Solid Freeform Fabrication Techniques

Fourligkas, N. and Doumanidis, C.
Tufts University, USA

Conventional thermal rapid prototyping techniques, such as laminated object manufacturing, fabricate 3-D geometry parts by material deposition or removal in successive 2-D layers, by using a localized heat source, such as a Laser beam. The sequential motion of this source on a trajectory dictated by the layer contours generates a highly concentrated temperature field, which exposes the material to thermal cycling often yielding an undesirable material structure and properties, and residual stress or distortion of a functional prototype. To address this limitation, a new scanned thermal actuation technique was recently developed to achieve independent, simultaneous control of multiple thermal quality features. In this method, the heat source reciprocates

rapidly over the entire layer surface, guided by an X-Y positioning system or robot, in a raster or vectored scanning motion. The torch is driven on dynamically scheduled trajectories, and its power is modulated in real time to provide a regulated heat input distribution on each layer. This scanned thermal actuation is determined in-process by a distributed-parameter control scheme, using temperature field feedback from an infrared thermometry camera, so as to obtain a specified thermal processing history and thus a desired material quality of the prototype.

Scanned thermal processing was modeled by an off-line numerical simulation of temperature field, featuring multiple moving grids, material deposition and/or removal, flexible multisource or continuous heat distributions, temperature-dependent material properties and latent transformation effects. A real-time, dynamic superposition description of the thermal field was also developed for scanned processing, based on spatio-temporal convolution of Green's fields. Numerical values of the Green's field were obtained by analytical conduction expressions, numerical simulation and direct experimental measurements, and were stored for fast in-process computation. Because of process nonlinearities and disturbances, the variable weighting factors of this superposition are updated by real-time parameter identification. Thus, this process description is used as a reference model in the design of an adaptive thermal control strategy.

This modeling has provided the basis for the development of an adaptive, distributed-parameter feedback controller of the torch power and motion for scanned thermal prototyping. The torch trajectories are dynamically defined to track the locus of the maximum deviation of the actual from the specified temperature field, thus guiding the heat source where its actuation is needed most. Several real-time thermal optimization strategies are developed, based on temperature hill gradients, flexible polytope patterns, Monte-Carlo sampling and weighted attraction methods. These are computationally tested on the numerical simulation as the process model, and experimentally implemented on a plasma-arc laminated object prototyping setup with thermal feedback from an infrared camera. This distributed-parameter adaptive thermal control system yields desirable material attributes together with the specified dimensional tolerances, and thus results in product quality and productivity advantages for thermal solid freeform fabrication.

Material Deposition Control In Thermal Solid Freeform Fabrication Methods

Kwak, Y.M. and Doumanidis, C.
Tufts University, USA

Most rapid prototyping methods employ heat for bonding of the material and/or cutting of the object layers, as well as for thermal treatment of the prototype. In addition, certain techniques use material addition from an external source (e.g. wire) onto a substrate, such as fused deposition modeling and ballistic particle manufacturing. In these methods, the prototype is developed by combined heat and mass transfer mechanisms, which determine the quality of the produced object. In particular, material deposition defines the dimensional features of the part morphology, while the thermal history during the process is responsible for the generated structure of the material and thus the mechanical properties of the object. However, the geometric distribution of molten material deposited on a solid layer clearly affects the heat transfer mechanisms and thus the temperature field in the latter. Also, differential thermal expansion of the material due to high temperature gradients often generates residual stresses and warpage distortions, a common concern in most techniques, which degrade geometric tolerances. Thus, the two process components, i.e. mass and heat deposition, are clearly interrelated and coupled.

This article establishes the modeling methodologies and experimental techniques for geometrical analysis of Rapid Prototyping processes with simultaneous heat and material deposition. In particular, a scan welding technique is used as a paradigm, in which a heat source, such as a plasma-arc torch or Laser beam, with simultaneous material addition e.g. in cold wire form, sweep rapidly the external surface of the developed part to deposit successive layers. These are generated by melting the external material thermally and fusing it to the already deposited metal in a continuous bead, which is properly meandered to compose a prototype slice of appropriate contours. The motion of the heat and mass source with respect to the part is provided by a generic process robot, or for axisymmetric prototypes by a special servodriven system translating the source with respect to a rotating part. Thus, solid freeform fabrication is implemented on a robotic plasma-arc processing station with wire feeding, with infrared temperature sensing and optical scanning of the surface geometry by the deflections of a Laser line.

The geometry of the melt surface is described by a linearized superposition expression, based on a time-varying unit deposition field identifiable by laboratory data. This deposition distribution, which is analogous to the Green's function in thermal conduction, is modeled by an ellipsoidal form, the parameters of which are updated by in-process identification. In addition, a lumped-parameter model is developed for these thermal and geometrical features of the molten puddle (i.e. width, height and temperature), on the basis of scalar mass, momentum and energy balances. The predictions of this computational model are compared to experimental measurements in elementary thermal and material deposition patterns, and provide the basis for off-line/in-process thermal-geometrical process control to obtain a desirable prototype morphology and material structure.

Session: D2-4 Room: Auditorium **Time: W3:30p-5:30p**
Chair: *J. M. Berg (Texas Tech)*

Advanced Automation Technology Needs and Applications in the Steel Industry

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DOFASCO Inc., Canada

The steel industry is under constant pressure from many alternate material suppliers (e.g. plastics, aluminum, etc.). All are competing to be the "material of choice" to the public. The demands are even greater for lighter, stronger, cheaper steels in light of todays highly competitive material market. Within the global steel industry, only those that can distinguish themselves from the rest meeting customer requirements will survive.

To compete, requires the need for the successful application of advanced control and modeling technologies. The complexities of the integrated steel production process provides many challenges in using advanced automation technology. Dofasco, one of North America's leading steel companies in the area of real-time process automation, has focused on the application of advanced control and modeling technologies at its plant in Hamilton, Ontario and will highlight these experiences in this discussion.

This presentation will focus on the special needs and challenges of applying advanced automation technology in the production of steel, especially noting where the academic community can provide help. Also presented will be a summary of situations where advanced control and modeling technologies have been successfully applied at Dofasco, with a specific example of an advanced real-time automation application. This specific example will highlight the application of a multivariate statistical model used in the control of Dofasco's iron desulphurization process. Using the technique "Projection to Latent Structures" (aka Partial Least Squares), an advanced statistical model was generated representing the relationship between the process data to the amount of reagent required to desulphurize the molten iron. The key deliverable for this system was to develop a new model-based control system that reduces process variations and thus reduce reagent use. This presentation will highlight the complexity of the problem from a process modeling point of view, the reason multivariate statistics technology is applicable, and the results of the application.

Bar Lapping Process Modeling and Control

Mei, Y. and Stelson, K.A.
University of Minnesota, USA

In the computer hard drive industry, the dimension of the "Stripe Height" (SH) of a recording head (or slider) is critical to recording density, hence it needs to be tightly controlled. This is achieved by the lapping process. Typically, the SH starts from several hundreds of micro-inches before lapping, and is lapped to about eighty micro-inches with a tolerance of ten to twenty micro-inches. An array of sliders are lapped simultaneously on the same bar. The initial SH distribution along the bar is typically non-uniform. The objective is to lap the sliders to a specified SH with as small variation as possible along the bar. The bar is then cut into sliders after lapping.

Lapping is achieved by first mounting the bar to a carrier. The carrier is pressed against a rotating lapping plate. Diamond particles are embedded on the surface of lapping plate. Meantime, slurry is distributed to the lapping interface. The combination of the resulting pressure and the relative motion between the bar and the lapping plate causes the bar material to be removed. Resistive lap sensors are fabricated along with the thin film heads to monitor the status of material removal at various locations.

During lapping, a dead weight is applied on the carrier-bar assembly. Another weight moves in the lateral direction while two thermal actuators bend the bar by thermal expansion. These three control actions adjust the lapping pressure distribution so that SH distribution is controlled.

A dynamic lapping process is established based on physical simulation. The Preston model is employed. It states that the material removal rate is proportional to the product of pressure and velocity. The beam on elastic foundation model is modified to account for non-flatness of surface in estimating the pressure. The physical simulation show good agreement with production observations. The lapping process model in state space form is then constructed semi-empirically and semi-analytically based on the pressure step response obtained from the physical simulation.

Open-loop solution of final SH from the identified state-space model are compared with that of the physical simulation. Results show that the open-loop solution is in general agreement with the physical simulation, indicating that the state space model is appropriate for closed-loop controller design.

A Level Set Framework for Calibration of Low-Order Etching and Deposition Models

Berg, J.M.
Texas Tech University, USA

This work is motivated by the need for accurate low-order phenomenological models of thin film etching and deposition processes. These processes are central to the manufacture of microelectronic devices. Phenomenological models are necessary because of the complexity of the surface chemistry and the plasma-surface interactions. Typically these models lump together numerous unknown rate constants into relatively few user-specified parameters. Reliable use of these models for simulation or control then depends

on the ability of the user to chose the values of these parameters correctly. One way to do this is to try to match the output of the simulation to surface evolution data from micrographs. However, there is no broadly applicable systematic procedure for accomplishing this. Previous work towards this end used a non-geometric cost function that required the user to select points in one-to-one correspondence on the actual and estimated surfaces. Such a requirement introduces an arbitrary component of unknown significance into the procedure, and places an undesirable burden on the user. This talk introduces a completely coordinate-free approach that eliminates this arbitrary element.

In a recent series of papers Sethian and Adalsteinsson apply level set methods to the simulation of feature development in a variety of semiconductor manufacturing applications. Level set methods provide a flexible framework for surface evolution problems. We apply this framework to the parameter identification problem. First we consider the problem of matching a parameterized level set function to a given zero level set. We show how our geometric cost function may be easily characterized and computed in terms of level set functions. We then construct and compute sensitivity derivatives. This allows us to apply the gradient descent class of minimization methods. A simple example is presented to demonstrate the principles. Next we consider how to proceed when—as in the calibration problem—it is not the level set function itself, but a corresponding speed function, that is parameterized. It is shown how to apply the Sensitivity Equation Method to obtain the necessary derivatives. The entire procedure is demonstrated on a simple example.

Feedback Control of Shape Memory Alloy Actuators

Dickinson, C., and Wen, J.T.
Rensselaer Polytechnic Institute, USA

Shape memory alloys are those materials which have the ability to "remember" their shape even after large deformations. Once deformed at a low temperature (in a martensitic phase), SMA will remain deformed until heated, when it returns to the original austenitic phase. SMA can be used as an actuator by coupling applied thermal energy to its internal phase transformation (between austenitic and martensitic phases) which in turn generates a mechanical strain. Because of their light weight and ability to produce large force and displacement, SMA have been used in a wide range of applications including large space structures, robotic arms, medical instruments, and surgical implants. SMA are commonly used with flexible structures for shape control, vibration suppression, and tracking control. However, there has been very little work done in controlling SMA mainly because they are assumed to be essentially static devices. In terms of open loop modeling of the SMA hysteresis, the Preisach model has often been chosen because of its simple structure, easy identifiability, invertibility, and implementability for both simulation and control. Recently, a passivity based approach has been used to analyse closed loop stability involving SMA, and a variable structure type of controller has also been successfully applied.

In this paper, we will describe our recent work on closed loop feedback compensation of SMA hysteresis. This paper builds on our previous work considering controlling a flexible beam with an externally attached SMA wire at the tip of the beam. We show that a simple nonlinear beam strain feedback control law can be shown to be stable under very general assumptions on the hysteresis model. In this control law, a static nonlinear map between the desired beam strain and a fictitious desired strain needs to be established experimentally. We further extend the control law to adaptively update the fictitious desired strain and obtain a general condition for stability by using the Circle Criterion. Experiments have been conducted to demonstrate the validity of our analysis.

Forging of A γ-TiAl Automobile Exhaust Valve Using Optimal Conditions

Mullins, W.M., Medeiros, S., and Fraizer, W.G.
Wright Paterson Air Force Base, USA
Smith, L.D., Kelly Air Force Base, USA
Berg, J.M., Texas Tech University, USA, and
Malas, J.C., Wright Paterson Air Force Base, USA

The processing of high-performance materials requires that both the final geometry and microstructure be carefully controlled. The complex deformation mechanisms and the strong coupling between deformation and microstructure evolution severely limit the freedom of the process designer in choosing feasible process parameters to produce a sound part. Recently an optimization technique, based on finite-element process simulation, was developed and used to determine the processing conditions required to produce an automotive valve preform. The results of the optimization predicted feasibility of the design and specified die geometry and processing parameters to produce a sound forging. This study describes an experimental verification of the optimization technique. A die-set was constructed and used to produce several sub-scale automotive valve preforms from a γ-TiAl alloy in a commercial, small-scale-production, isothermal forge press. The results of the forging experiments demonstrated the feasibility of the initial design, as predicted by the optimization technique. In addition, the experiments highlighted the importance of several processing parameters that were not included in the original models, but that can dramatically affect the commercial viability of a process.

Symposium E1
Mechanics, Micromechanics and Processing of Composites and Ceramics
Organizers
I. Demir, King Saud University, Saudi Arabia
M. Garnich
Pacific Northwest National Lab, USA
&
M. Khraisheh
King Fahd University, Saudi Arabia

Session: E1-1 Room: CUB 222 **Time:** T3:30p-5:30p
Chairs: *M. Garnich (PNNL) & M. T. Smith (PNNL)*

A Multicontinuum Approach to Structural Analysis of Linear Viscoelastic Composite Materials

Garnich, M.R. , Pacific Northwest National Laboratory, USA and
Hansen, A.C. , University of Wyoming, USA

This paper centers on a unique approach to the analysis of the deformation response of composite structures. The approach is based on a theory and associated numerical algorithm for extracting, virtually without a time penalty, the stress and strain fields (in the continuum sense) for the constituents of a composite in the course of a routine structural Finite Element Analysis (FEA). The finite element implementation is referred to as Multicontinuum Theory (MCT) which reflects the coexisting continuums within a typical composite material. MCT is an enabling technology that provides the analyst with a window on the behavior of a composite structure at its most basic level, i.e., the individual constituents.

The multicontinuum theory has been developed for the case of a linear elastic reinforcing material with a linear viscoelastic matrix material. Finite element micromechanics is used to establish relationships between the composite and constituent field variables. The micromechanics analysis is a one time preprocessor to a structural solution and hence does not impose a computational penalty on the structural analysis.

The paper will present the theory behind the multicontinuum analysis along with time history results for a variety of thermal-mechanical load conditions applied to a viscoelastic unidirectional composite material. MCT results are verified by comparing the solutions with constituent stress and strain fields generated in a traditional finite element micromechanics analysis.

Functionally Designed Metal-Ceramic Composites Via Solid Freeform Fabrication

Diaz, M.R. and Bandyopadhyay, A.
Washington State University, USA

Solid Freeform Fabrication (SFF) is a relatively new approach in the prototyping and manufacturing arena, which gained a significant interest in recent years due to its inherent flexibility in manufacturing simple and complex geometry parts without any part specific tooling, molds or dies. SFF is an approach to directly build three dimensional components layer-by-layer from a computer data description or a CAD file of a component. In this work Fused Deposition (FD) process is used where a thermoplastic polymer filament passes through a heated liquifier, and liquifier extrudes a continuous bead, or road, of material through a nozzle and deposits it on a fixtureless platform based on CAD file of the part.

The concept of Functionally Designed Materials (FDM) is somewhat similar to the functionally gradient materials where the composition in a composite is inhomogeneous and may change from one extreme to the other. Functionally designed materials can be designed based on its functionality using computer aided design (CAD) software. These structures can then be fabricated using advanced processing techniques such as SFF. In the case of functionally designed metal-ceramic composites, some areas might be ceramic matrix composites and some other areas might be metal matrix depending on its functionality.

In this work, indirect SFF process is used, where a polymeric mold with the negative of the desired structure is fabricated via SFF. The mold is infiltrated with silica slurry, dried and then the structure is subjected to a binder burn out and sintering cycle to produce a sintered porous silica preform. Sintered porous silica ceramic preforms are then infiltrated with different Al alloys. During metal infiltration, Al replaces Si in the ceramic preform and forms alumina (Al_2O_3), which results an aluminum/alumina composite.

In this presentation, processing of porous silica preform via SFF, and effects of various alloying elements on the phase transformation kinetics to form Al/Al_2O_3 composites will be discussed.

Net Shaped Al_2O_3/Bioglass Composites for Orthopedic Applications

Hanabe, M.H., Khasbardar, V. and Aswath, P.B.
University of Texas at Arlington, USA

A major uses of ceramics in the biomedical industry is in orthopedic applications in the form of implants, prosthesis or prosthetic devices. Clinical success of implants require a simultaneous achievement of a stable interface with the connective tissue and a proper match of the mechanical behavior

of the implant with the tissue. Coupled with these two biomedical issues is the practical problem of making feasible implants tailored for individual patients in a short time.

Al_2O_3/Al composites were synthesized by reactive infiltration of molten Al into preforms of solid SiO_2 1075° C. Displacement reactions between and Al lead to *in-situ* formation of the composite and also aids the infiltration of the melt.

On completion of the reaction the preform is withdrawn from the melt and it is a composites which have a three dimensional network of channels of Al and Al_2O_3. The exact shape of the preform is retained yielding a near net-shaped Al_2O_3/Al composite. In the presence of Mg, it was found that the consistency of infiltration was better and that the transformation of silica to alumina involved intermediate displacement reactions unlike the single step reaction without Mg in the preform. It was observed that the morphology and size scale of the composite Al_2O_3/Al were affected by the presence of Mg. Without Mg a finer scale Al_2O_3/Al microstructure which had a tendency to be elongated in the growth direction was formed, while a coarser morphology with interconnectivity in both the phases developed from Mg + SiO_2 preforms.

Once the composite is formed, Al is leached out leaving behind a porous Al_2O_3 structure which is now the preform for the infiltration of Bioglass. The product is a Ceramic-Glass composite with three dimensional interconnectivity of both Al_2O_3 and Bioglass.

Research supported in part by the State of Texas by an Advanced Technology Grant.

Modelling of Mechanics of Composites by Electrical Analogies

Szekeres, A., TU of Budapest, Hungary

Both the thermal and hygroscopic features are basic properties of composites that appear very often cross-coupled. They are associated manyfold.

First, the analogy between Fourier's and Fick's laws gives a wide possibility for the common analytical, numerical and experimental handling of thermal and moisture fields in composites [1]. Second, there is a cross-coupling between these fields due to Soret and Dufour effects [2]. Third, both cause degradation in composites which may lead to failure [3]. Fourth, both effects are told to be only environmental ones [3,4], which is not valid. In dynamical cases, e.g. according to the Gough-Joule, Soret and Dufour effects the displacement, thermal and moisture fields are always coupled, in spite of the smooth environment.

All of these show the difficulties when dealing with thermo-hygro-elastic composites, e.g. with tailoring. The electrical analogy gives a special tool by which one gets

-- deeper insight of the problem,

-- analytical method for solving the complicated differential equation system,

-- numerical possibility based on this and

-- experimental method to model the problem [5].

Based on the above we display the results of electrical analogies in coupled fields of mechanics and their application to tailoring of fiber reinforced composites.

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Determination of Glass Transition Temperatures of Adsorbed Stereoregular PMMA by Inverse Gas Chromatography at Infinite Dilution

Hamieh, T., Rezzaki, M. and Schultz, J.
University of Alberta, Canada

In this paper, we used inerse gas chromatography (IGC) at infinite dilution to determine glass transition and other transitions of poly methyl methacrylate (PMMA) adsorbed on alpha-alumina at various covered surface fractions. The study of the chemical physical properties of PMMA/Al2O3 revealed an important difference in the acidic and basic behaviour in Lewis terms of aluminum oxide covered by various concentrations of PMMA. We also highlighted an important effect of the tacticity of the polymer on the acidic basic character of the system PMMA/Al2O3.

Session: E1-2 Room: CUB 222 **Time:** W9:30a-11:30a
Chairs: *L. V. Smith (WSU) & I. Demir (K. Saud U)*

Residual Stresses in Embedded Fiber Optic Bragg Gratings

Christiansen, M.B. and Koh, S.L.
University of Maryland Baltimore County, USA

Fiber optic sensors provide a technique for measuring strain inside laminated composite materials. The fiber optic Bragg grating measures strain,

temperature, and other physical parameters. It encodes the needed information via wavelength rather than optical phase changes as done in the interferometric sensors, e.g. Fabry-Perot. Inserting a Bragg grating during the manufacture of a composite material produces residual stresses in the optical fiber that must be taken into consideration in the use of the sensor. Thermal expansion of the epoxy matrix is more than ten times larger than either the glass or carbon fibers. Residual stresses produced during cooling result in large internal stresses in the composite. The fiber optic Bragg grating in shear allows for independent measurement of both mechanical strain and temperature (Dunphy, 1995). A finite element analysis shows the relationship between re-enforcing fibers, epoxy matrix, and the fiber optic sensor. These finite element results are compared with results from a photoelasticity experiment.

Factors Affecting Fiber-Matrix Bond Strength Determination In Composites

Kahraman, R. and Mandell, J.F.
King Fahd University, Saudi Arabia and
Sahin, A.Z., Montana Sate University, USA

The fiber-matrix bond strength appears to be the most important interfacial property that is known to influence the bulk composite properties. The technique used to measure this interfacial property in this investigation is based on a microdebonding test method and apparatus developed by Mandell et al.. Originally developed for polymer matrix composites, this indentation technique has also been applied to metal, glass, and ceramic matrix composites. The microdebonding test yields a measurement of the shear strength at the fiber-matrix interface. To be able to correlate composite behavior with the properties of fiber-matrix interfaces, this interfacial property must be accurately measured. The objective of this study was to examine the factors influencing such measurements.

The materials used in this study were mainly AS4/Epoxy 3501 (a polymer matrix composite) and Nicalon/CAS-II (a ceramic matrix composite). However, the repeatability of the results were also checked on several other composites.

The specimens consisted of composite laminates which have been sectioned perpendicular to the reinforcing fibers and potted in an epoxy compound in plastic casting cups. The embedded length was about 1 cm. Grinding and polishing of the mounted specimens were performed on a metallographic polishing bench using a series of Struers silicon carbide grinding papers and Buehler alumina solutions with rayon bonded to cotton cloth or diamond slurry suspension with lapping oil on silk cloth. Specimens to be tested were mounted (pressed) on the test stage using plasticene.

Fiber-matrix bond strength (the maximum value of the interfacial shear stress at the initiation of debonding) measurements were done using the indentation technique, where individual fibers are compressively loaded in steps of increasing force (by a ground diamond tipped probe) on a polished surface until debonding is observed optically between steps. The microdebonding testing system was a modified version of the one originally developed by Mandell et al. It had two major assembly stations which are the microscope (with a magnification of 1000×) and microindentation station on a vibration isolation table and the auxiliary monitor and printer station.

First the probe position is adjusted until the location of probe contact on the specimen is observed through the monitor. At the microscope station fibers are selected and located for testing, and observed after each loading step for evidence of interface failure. Debonding appears usually suddenly over part of the fiber circumference at a particular load level. The specimen is on a conventional rotating stage with magnetic stops at the viewing and loading stations. The load is applied by raising the specimen against the probe using the vertical component of the x-y-z stage and measured through a load cell attached above the probe. The load is maintained at the desired level of each loading step for some time and increased by a small amount after observation of the fiber tested.

The bond strength of the fiber-matrix interface is then calculated by utilizing a finite element analysis code. A simplified axisymmetric geometry was employed to model the stress field generated by the probe loading. The model consisted of the fiber, surrounding matrix material of constant thickness and averaged composite properties beyond the matrix. Linear elastic behavior was assumed and thermal residual stresses, which develop during processing when the composite is cooled down from the solidification temperature, were included in the analysis. The significant findings of this investigation are as follows:

1. Suggested surface preparation sequence for polymer matrix composite specimens is grinding with 800, 1000, 1200, 2400 and 4000 grit silicon carbide paper followed by polishing with 0.05 μm alumina solution.
2. Suggested order of polishing for ceramic matrix surfaces for microdebonding analysis is grinding by 320, 500 and 800 grit silicon carbide papers followed by polishing with 15, 9, 6, 3, 1 and 0.25 μm diamond solutions.
3. In the case of surfaces polished in lapping oil, the surface should be cleaned well at the end of polishing and care should be taken not to interpret the oil at the edges of a fiber during loading as debonding.
4. Testing fibers with similar geometry gives best results.
5. The reliability of the measurements might be affected if the area contacted by the probe approaches the fiber circumference within a distance less than 1 μm.

The Effects of Moisture on the Fatigue Response of Polymer Matrix Composite Materials

Smith, L.V.
Washington State University, USA

The presence of moisture is known to affect the mechanical response of polymer matrix composite materials. Moisture can relieve processing induced residual stress through matrix swelling as well as degrade strength, stiffness, durability and accelerate time dependent behavior. This study examines the effect of moisture on the fatigue response of composite materials. Dry and saturated coupons were tested in air and while immersed. The effect of moisture was reconciled by comparison with dry coupons fatigued in air. Experimental results showed that saturated coupons fatigued in air exhibited an extended fatigue life over dry coupons. The beneficial properties of saturation are likely related to stress relief from moisture related swelling. Coupons fatigued while immersed exhibited a reduced fatigue life and increased delamination. It was postulated that the degraded fatigue life observed during immersed fatigue was related to moisture entering transverse cracks, which formed during dynamic loading. The observed behavior was examined using a shear lag model and finite element analysis. By considering the disparate time scales of moisture sorption, capillary flow and load fluctuations, these static models are able to show the combined effects of moisture and dynamic loading on the coupon stress state.

Effects of Fiber Coating on Tensile Properties at High Temperatures of Boron-Aluminum Composites

Liu, S-J., Tang, R-S. and Shun, C-Y.
Beijing Institute of Aeronautical Materials, China

In present study, effects of fiber coating on longitudinal tensile strength behavior of B/A1$[0]_6$ laminate composite was investigated experimentally at room temperature and several temperature ranges of 200,300,350,400 °C, respectively.

Materials:
B/A $[0]_6$ laminated composite
Fiber --- Boron Fiber
Matrix --- Aluminum alloy
Volume fraction $V_r = 0.5$

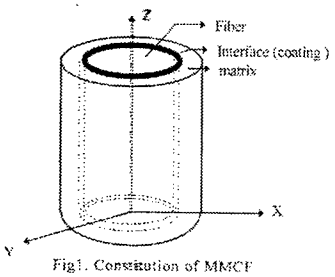


Fig1. Constitution of MMCF

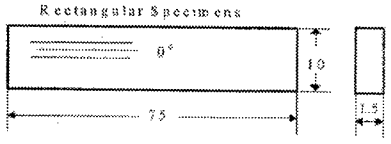


Fig2. Specimens

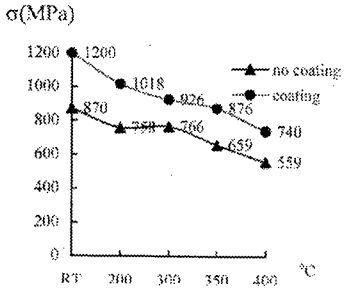


Fig3.effect of fiber coating on tensile strngth

The conclusions based on tensile testes of B/A1 composites are summarized as follows:

1. Fiber coatings greatly improved the tensile properties.
2. The tensile strength of B/A1 laminate composites with fiber coating was 1.3 times as large as those without fiber coatings at room temp, 200, 300, 350 and 400 °C, respectively. (see Fig. 3).
3. B/A1 laminate composites with fiber coatings showed cyclic hardening behavior, but without fiber coatings showed cyclic sorting behavior.

Mechanical Properties of Tungsten-Silica Composite

Jia, D. and Ramesh, K.T.
Johns Hopkins University, USA

The Mechanical properties of a tungsten-silica composite have been investigated at different strain rates ($10^{-3}s^{-1}$ – $10^{+3}s^{-1}$) using a servohydraulic system and a compression Kolsky bar respectively. High-strain-rate experiments have also been performed over the temperature range of 300 - 700°C on this composite. Stress-strain curves for the investigated materials, which contains 98.2 wt% W, 1.5wt% SiO_2 and 0.3 wt% Ni, are obtained in compression. The results of the different strain rate tests show that the yield stress is rate-sensitive, while the strain hardening is not strongly rate dependent. The temperature dependence of the yield stress of the composite is approximately the same as that of pure tungsten. However, strain softening is observed when the temperature is over ~600°C, which is caused by the glassy inclusions (SiO_2) with low thermal conductivity

and low glass transition temperature. The deformation and failure mechanisms of the material operative at low and high strain rates are analyzed using optical and scanning electron microscopy (SEM). The observed behavior of the W-SiO_2-Ni composite is compared with the predictions of numerical modeling.

Session: E1-3 Room: CUB 222 **Time:** W1:00p-3:00p
Chairs: *M. Khraisheh (K. Fahd U) &*
A. C. Hansen (Wyoming)

Analytical Determination of Plastic Deformation During Continued Cyclic Loading of Composite Spheres and Cylinders

Bhattacharyya, A. and Appiah, E.J.
University of Alberta, Canada

The stress-strain response under continued cyclic loading is analytically determined for the following two configurations: (a) an inclusion-matrix concentric sphere subjected to cyclic hydrostatic loading, (b) an inclusion-matrix concentric cylinder subjected to plane strain, cyclic biaxial loading. In either case, a bilinear matrix is assumed and yielding is assumed to occur in the matrix by the vonMises' criterion. Purely kinematic hardening and purely isotropic hardening are separately considered, as limits of the work hardening nature of a matrix material. Based on Hill's (1950) approach, the exact solution is determined for the aforementioned configurations for the first 3 cycles of loading (or 6 loading and unloading sequences). Based on this exact solution, the analytical relation between the overall stress and strain at the *n*th loading cycle is *suggested*. The theoretical approach is finally validated by comparing the analytical results for the concentric cylinder model with finite element computations.

1. Hill, R. The Mathematical Theory of Plasticity, Clarendon Press, Oxford, England, 1950.

Natural Vibration Characteristics of Rotating Adhesively Bonded Cantilever Plates

Yavuz, A.K., and Kotil, T.
Istanbul Technical University, Turkey

In this study, free vibration analysis of rotating adhesively bonded cantilever isotropic thin plates is investigated. In the analytical model, the thin interlaminar adhesive layer are taken into account in the form of compression-tension and shear springs with spring elastic constants approximating adhesive elastic characteristics. Application of Ritz method is done by using beam functions in a special form as trial functions so as to predict the free vibration frequencies and corresponding mode shapes of the system under consideration. Mode shapes are plotted and extensive parametric studies are performed.

A Rigorous Theory for the Elastostatic Analysis of Laminated Beams

Abduljabbar, Z.S.
King Saud University, Saudi Arabia

Aside from the exact elasticity solutions, all the existing beam theories resort to ad hoc assumptions to simplify the exact equations. Consequently, certain aspects of exactness are deemed to be violated rendering each theory inadequate for certain applications due to loss of accuracy. In particular, in the analysis of laminated beams the search for a rigorous theory is justified by the need to satisfy the interlaminar continuity of tractions and displacements. Such a condition necessitates accurate modeling of through-thickness variation of the relevant variables.

This paper presents an asymptotically exact beam theory derived on the basis of the theory of elasticity without the classical unfounded assumptions. The derivation exploits the slenderness of beams and employs the technique of parameter perturbation to reduce the governing equations to a simple form that complies with all the conditions of the exact theory. However, due to the so-called edge effect, the imposition of the boundary conditions on the ends of the beam involves tedious mathematical manipulations. In the present paper, for the sake of preserving simplicity, we utilize a least-square technique to satisfy the ends boundary conditions in an approximate sense. This is achieved by minimizing the relevant boundary residuals. Accurate treatment of the edge effect will be addresses in a future paper.

The theory is presented in a two dimensional form. The results reveal that the beam stresses and displacements can be represented by power series expansions in terms of the thickness to length ratio. The leading terms in the expansions are found to be of resemblance to the stress and displacement fields of the Bernoulli-Euler beam theory. The higher power terms reveal the effects of the transverse normal and shear stresses. The methodology can be employed in the three-dimensional analysis of composite anisotropic beams of rectangular cross section. However, this would necessitates the adoption of double power series expansions in terms of the thickness to length ratios. Similar theories can be derived for the analysis of laminated anisotropic plates and shells.

Synthetic Constitutive Data for Random Composites

Aidun, J.B., Lo, D.C.S. and Rintoul, M.D.
Sandia National Laboratories, USA

For numerical simulation of structural response it is often useful to approximate the behavior of a random composite by an equivalent homogeneous material. Use of a homogenized material model for a heterogeneous composite carries with it two requirements to insure acceptable accuracy. One is

defining meaningful effective overall properties to describe the inelastic or nonlinear response of the homogenized material. The other is identifying the minimum size for which the homogenized model approximation provides the desired accuracy. Alternately stated, the latter requirement is to determine the representative volume (RV) of the heterogeneous continuum and insuring that the relevant regions in the numerical simulation equal or exceed this size. The application of interest at SNL is to use detailed, fine-scale finite element method solid mechanics simulations of the mechanical response of specimens of a random composite to generate synthetic constitutive "data" and combine it with laboratory measurements to develop a homogenized material model. Materials of interest include filled (particle-impregnated) epoxy and microcracked ceramic. The RV size is of basic importance to this undertaking. The simulated specimens must be at least as large as the RV for simulated volume-averaged response to be representative of the macroscopic behavior of the composite. Previous preliminary work on an elastic matrix with periodically arranged elastic spherical inclusions established the accuracy of the numerical tools to be within 10% of theoretical values with typical agreement being better than 4%. We will present recent progress in developing techniques for determining the RV size for selected random composites. We will also discuss concepts to guide the definition of effective properties for nonlinear and inelastic material response.

*Sandia is a multi-program laboratory operated by the Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AL04-94AL8500.

Structural Response of Laminated Composite Shells Subjected to Blast Loadings

Türkmen, H.S. and Mecitoğlu, Z.
Istanbul Technical University, Turkey

This paper is concerned with the theoretical analysis of the cylindrically curved laminated composite panels exposed to normal blast shock waves as well as presenting correlation between the theoretical analysis and the experimental results of the strain-time histories. The laminated composite panel is clamped at its all edges. On the theoretical side of the study, dynamic equations of the cylindrical shell are derived by the use of the virtual work principle within the framework of Love's theory of thin elastic shells. The governing equations of the cylindrically curved laminated shell are solved by the Runge-Kutta-Verner method. On the experimental side of the study, the cylindrically curved panel tests have been carried out on the laminated composite shells with clamped edges for various blast loadings. For obtaining the air blast loading a detonation wave is developed from the reaction of LPG – Oxygen mixtures in a long circular cylindrical shock tube. The detonation wave goes through into the atmosphere from the open end of the shock tube and act as a blast load on the panel, which is placed in front of the shock tube. Mounting of the target panel on a steel frame is designed with the object of providing clamped boundary conditions. The air blast pressure distribution is obtained by the use of a quartz crystal pressure transducer placed on the wooden model. Strains are measured at the center of the panel. Furthermore, a finite element modeling and analysis are presented and experimental results are compared with the results of theoretical method and finite element analysis. As well, the effects of loading conditions, geometrical properties and material properties are separately examined on the dynamic behavior. In the longitudinal direction of the cylindrical panels strain-time history curves show that an agreement between the experimental and analyses results. In the circumferential direction of the cylindrical panels there is a discrepancy between the experimental and analyses results because of using the inadequate number of terms in the theoretical analysis. If the frequencies are considered, an agreement is found between the experiment and analyses results for cylindrical panels.

Symposium E2
Compressive Failure in Fiber Composites
Organizers
T. Waas
University of Michigan, USA
&
C.R. Schultheisz
National Institute of Standards and Technology, USA

Session: E2-1 Room: Cascade 127 **Time:** M10:00a-12:00p
Chairs: *A. Waas (U. Mich.) & C. R. Schulteisz (NIST)*

A Critical Review of Concepts Used to Explain the Compressive Properties of Fibre Composites

Piggott, M.R.
University of Toronto, Canada

Compressive failure is complex, involving a diversity of possible processes. Unfortunately, simplistic treatments abound, and some have proven to be durable, in the composites literature at least, despite not agreeing with experimental data. These include the theory of Rosen which should be regarded as suitable only for perfect composites, and the theory of Argon which appears to have been based on a misunderstanding of early experimental results. Some modern theorists manage to combine Rosen and Argon, but the old adage about computers and garbage should be borne in mind here. Real composites are imperfect, involving wavy fibres, imperfectly packed, and in some cases, imperfectly bonded to the polymer. Some fibres are weak in compression (especially polymer fibres such as Kevlar and Spectra). The polymer matrix has no shear failure mode, nor does it have a compressive failure mode, at least with respect to total separation. Thus ultimate failures must be due to the fibres themselves, or to the introduction of transverse tensile stresses associated with the imperfections. Fortunately, we now have methods for quantifying the imperfections. What is presently needed are more definitive studies linking the compressive strength of unidirectional fibre composites and the imperfections therein. Theorists should take a back seat until good data on this is available. Meanwhile, they might find it interesting to search out the original papers, and read them carefully.

Nonlinear Viscoelastic Effects in the Compressive Strength of Unidirectional Fiber Composites

Schapery, R.A.
The University of Texas at Austin, USA

The compressive strength of a unidirectional composite ply in the fiber direction is commonly limited by a local shear instability; the fibers rotate and the matrix undergoes significant shearing, usually leading to the kink bands observed in failed specimens. This shear-type instability can be expected when the axial modulus of a ply is much larger than the principal shear modulus. In this talk I discuss nonlinear viscoelastic constitutive equations for fiber composites and their application to the compressive strength problem. Specifically, experimental and theoretical results are described for a continuous carbon fiber composite with a rubber-toughened epoxy matrix.

As part of an experimental program, nonlinear viscoelastic material constants and functions were determined and validated from a series of experiments at several temperatures, using constant load rate and creep and recovery tests. Compressive failure times in creep and in constant load rate tests at several temperatures were also obtained for this material. With these results it is shown how failure may be predicted using a master strength curve as a function of reduced rate or time, and how this curve is related to the initial fiber waviness.

Schapery, R.A. (1993), "Compressive strength and failure time based on local buckling in viscoelastic composites," Appl. Mech. Rev. Vol. 46, S221-228.

Schapery, R.A. (1997), "Nonlinear viscoelastic and viscoplastic constitutive equations based on thermodynamics," Mechanics of Time-Dependent Materials, Vol. 1, 209-240.

Research in Composites for Marine Structures: ONR Perspectives

Rajapakse, Y.D.S.
Office of Naval Research, USA

Composite materials provide many attractive options in the design and utilization of affordable and reliable naval structures. Current research thrusts on "Composites for Marine Structures" in the Ship Structures and Systems S&T Division at the Office of Naval Research address a variety of fundamental issues of composite ship structures in marine environments. Affordability is an over-riding concern in the large scale use of composites (e.g. ship structures). A major focus is on polymer matrix composites, with increased emphasis on affordable composite systems, including resin transfer molded composites and sandwich structures. Other drivers include survivability, reliability, structural integrity and durability.

The objective of these thrusts is to establish the thermo-mechanical behavior and radiation response of polymer matrix composites and composite sandwich structures, subjected to multiaxial static, dynamic and cyclic loading in severe environments, including extremes of temperature, moisture, sea water, hydrostatic pressure and radiation fields. A balanced approach of advanced experimental techniques, theoretical analyses, and computational methods, is used in the elucidation of the physical processes

involved, and in the establishment of quantitative models capable of predicting the behavior of composite structures in the marine environment. These structures include multi-functional multi-layered composite systems, integrating structural composites and signature reduction material systems.

An overview of current research and scientific accomplishments will be provided in the presentation. Topics discussed will include: moisture/sea-water effects, three-dimensional constitutive equations, dynamic constitutive equations, strain rate effects, hydrostatic pressure effects, failure modes and failure criteria, compression failure, structural failure modes, coupling between material and structural failure, multi-functional sandwich structures, and response of composite structures to dynamic/shock loading.

Session: E2-2 Room: Cascade 127 **Time:** M1:30p-3:30p
Chairs: *Y. Rajapakse (ONR) &*
R.A. Schapery (U. Texas-Austin)

Dynamic Compressive Behavior of Glass Fiber Reinforced Unidirectional Vinyl Ester Composites

Waas, A.M. and Lee, S.H.
University of Michigan, USA
Takeda, N. and Yuan, J.M.
University of Tokyo, Japan

The effect of fiber volume fraction and fiber mechanical property on the static and dynamic compressive strength of fiber reinforced polymer matrix composites is investigated. Investigations that examine the dynamic tensile and compressive behavior of such composites is relatively scarce compared to static experiments. In this presentation, results obtained from an experimental investigation pertaining to the static and dynamic compressive strength of unidirectional glass fiber and carbon fiber reinforced polymer composites will be presented. A SHPB (Split Hopkinson Pressure Bar) is used to investigate the dynamic compressive response. The dependence of dynamic compressive strength on fiber volume fraction is investigated. The dynamic compressive behavior of the pure matrix(vinyl ester) is also investigated for purposes of comparison. The specimens are of circular cylindrical shape with nominal length of 12.7 cm. Fiber volume fractions range form 10% to 60%. Several trials of similar specimens consist of dynamic compression at nominal strain rates of 200/sec-1500/sec. Strain data are collected via strain gages placed on the incident bar and transmission bar as well as on the specimen surface. In this manner, the accuracy of the data can be checked by using information from all strain gage outputs. Splitting and Kink Banding are found to be the dominant failure mechanisms. These modes operate alone or as a combination, effected by fiber type, fiber volume fraction, strain rate and initial fiber misalignment. The dynamic results are examined in the light of corresponding static tests for similar specimens. In this manner, by controlling the type of fiber and the fiber volume fraction whilst maintaining the same matrix material, it becomes possible to isolate the influence of fiber mechanical property on the measured compressive strength. The splitting and kinking modes are modeled via a simple fracture mechanics based model and the finite element method is used to understand the kink banding mode of failure. Excellent agreement between experiment and analysis is reported.

Mixed-Mode Stress Intensity Factors For Composite Plates with Single Delamination Under Compression

Huang, H. and Kardomateas, G.A.
Georgia Institute of Technology, USA

Under compression, the structure with delamination may buckle and cause the delamination to propagate. According to the post buckling analysis of a delaminated composite plate under compression, the internal compressive forces and moments at the intersection of the delamination tip indicates that the delamination is subjected to mixed-mode loading. Therefore, an extensive research is needed to gain insight into the factors that influence the mode I and mode II stress intensity factors, which in turn control the delamination onset and growth. The local crack-tip geometry of the orthotropic plate is idealized as a semi-infinite plate with a crack perpendicular to its edge. An analytical method based on the continuous dislocation technique and conformal transformation is developed to calculate the mixed-mode stress intensity factors around the crack tip of an anisotropic semi-infinite strip subjected to edge forces and moments. To overcome the difficulty of calculating the stress distributions in the semi-infinite strip due to dislocation and edge loading, the semi-infinite plate is transformed into a half plane, on which the stress potentials due to external loads and dislocations can be obtained. Continuous dislocation technique is then employed in the half plane to calculate the dislocation densities and crack tip stress intensity factors, which are related to those of the semi-infinite strip. Combining the post-buckling analysis and stress intensity factor calculation, the delamination growth characteristics of composite plates under compression are discussed. It is found that the delamination growth is dominated by mode II loading. When the delamination locates close to the free surface of the plate, it grows under pure mode II condition. In addition, the stability of the delamination propagation is also discussed. Under constant end-shortening condition, the delamination growth is unstable when the delamination is short and stable when it is long.

On the Determination of Strain Energy Release Rates in 2-Dimensional Delamination Buckling Scenarios

Johnson, M.J. and Sridharan, S.
Washington University, USA

Various approaches to the determination of the energy release rate (G) are critically reviewed. These are : J -integral , crack-closure integrals and the direct method of integrating load-end compression (P- Δ) relationships. Of these J-integral which is based on the assumption of small displacements is shown to be a poor approximation for the delamination buckling problems. The crack-closure integral which provides modal contributions (G_I and G_{II}) is studied for cracks between plies having the same and different material properties respectively. Interestingly, for laminated composites, these integrals do converge as the finite element discretization is made finer, in the face of theoretical finding that they do not converge. However the calculations depend on stress distributions in the vicinity of the crack tip and require computational effort which is an order of magnitude higher than that required for routine structural analysis. In contrast, the total energy release rate, G, obtained by the integration of P-Δ relationship is highly robust and is accurately found using a coarse mesh. This is a displacement-based approach and does not depend on crack-tip stresses.

Authors propose a new displacement-based method for determining the modal components, G_I and G_{II}. The values obtained by this method are slightly lower than those obtained by the stress-based approach, but because they are not dependent on a description of crack-tip stress field, they are robust and converge at a much faster rate and exhibit the same trends of variation with the load. This approach is expected to prove valuable from the point of view of prediction of crack-growth.

The effect of material degradation on G is studied using a micro-model. The material degradation considered was an "overall" one in that the localized material damage in the vicinity of the crack tip was not modeled in detail. The effect, then, was one of increase in the strain energy release rate with material degradation. This is the result of loss of stiffness and increased deflection at the structural level.

Methods presented in this work were verified against experimental data available in literature. Currently used crack-growth criteria are critically reviewed.

The work includes a study of multiple delaminations (in series and parallel) as a scenario to be considered in the design of compressively loaded laminates. It is demonstrated that cracks in series do not tend to coalesce, but if at all, tend to grow away from each other. Multiple parallel cracks are not necessarily more critical than a single crack in compressively loaded laminates.

Failure of Laminated Composites at Thickness Discontinuities Under Complex Loading and Elevated Temperatures

Lee, S. and Knauss, W.G.
California Institute of Technology, USA

Failure initiation of laminated composites with discontinuous thickness has been studied in terms of typical structural load description (tension, shear force and bending moment) rather than in terms of micromechanics considerations. Four types of specimens of different stacking sequence were examined to determine failure initiation, analyzed subsequently via a finite element analysis (ABAQUS). Depending on the stacking sequence across the interface of the step, two different failure modes are identified: For uni-directional fiber orientation across the interface in the tension direction failure occurs through cracking and delamination which is governed by a fracture mechanics criterion. While the initiation strength for this failure mode is higher than for the cross-ply configurations, the residual strength after initiation is only marginally higher, providing virtually no margin of safety. For cases involving cross-plies on either side of the interface, failure initiation occurs by matrix cracking, with a critical strain across the fibers providing a universal failure criterion. In these cases the residual load bearing capability was 20 to 30% higher than the failure initiation loads. The interaction between moment and tension at failure initiation is linear, an observation that does not hold for the delamination failure driven by crack propagation. Assuming that time dependent aspects of the failure process are not dominant, elevated temperatures did not change the general results of how bending and tension loads interact, provided one accounts for residual thermal stresses; however the magnitude at which the failures occur depends on the temperature.

Buckling Simulations of Composite Sandwich Panels With Core to Face Delaminations

Riks, E.
Delft University of Technology, The Netherlands, and
Rankin, C.C.
Lockheed Martin Missiles and Space, USA

Current finite element models of sandwich structures are usually based on two dimensional theories whereby the study of the deformation of the three dimensional sandwich structure is reduced to the study of the deformation of a two dimensional reference surface with special properties. This approach, which corresponds to the computerization of the classical sandwich theory, is rather restricted and does not fully exploit the potential that the finite element codes provide.

In this paper we propose a different approach. It results in a more versatile model with several features that the classical model cannot offer. This new model views the sandwich as a composite structure consisting of a three dimensional core complemented with two dimensional shell faces.

Following this concept the faces are modeled by existing nonlinear shell elements while the core is modeled by adapted volume elements, thus creating an improvement in behavior that far exceeds the classical models. The improvements are not only in the area of the boundary conditions, always a difficult point in the classical approach, but also in the area of the description of local effects such as local buckling of the faces and delamination buckling.

The model, which is now part of the STAGS code [1], is geometrically nonlinear with no restrictions on the size of the rotations. The faces are represented by a general laminate theory while the core is thought to have general homogeneous anisoptropic elastic properties. Taken together, these features make it possible to represent the behavior of a wide range of sandwich configurations that are used in airframes and other light weight constructions.

To demonstrate the capabilities of this model we considered the simulation of the buckling and postbuckling behavior of a sandwich with a partial delamination between core and face, or a delamination in one of the composite faces, a problem that is of considerable interest for the assessment of the residual strength of the sandwich compression panels. It will be shown that apart from the contact problem, it is also necessary to overcome the difficulty that mode jumping is a pivotal element in the postbuckling behavior of the panel.

[1]. Rankin C. C., Brogan F.A., Loden W. and Cabiness H., Structural Analysis of General Shells, STAGS, User manual, version 3.0, LMMS P032594, Advanced Technology Center, Lockheed Martin, Febr. 1998. Palo Alto, California.

Session: E2-3 Room: Cascade 127 **Time:** M4:00p-6:00p
Chairs: *W. S. Slaughter (U. Pittsburgh) & G. Ravichandran (Cal. Inst. Tech)*

Buckling And Failure of Axially-Loaded Elliptical Composite Cylinders

Hyer, M.W.
Virginia Polytechnic Institute and State University, USA and
Meyers, C.A.
Materials Sciences Corporation, USA

Finite-element numerical results and experiments were used to study the response of a series of small-scale composite cylinders with elliptical cross-sections to axial end shortening. Nine eight-ply graphite-epoxy cylinders, three lay-ups for each of three cross-sectional aspect ratios, were fabricated from Hercules AS4/3501-6. The nominal semi-major axis for all specimens was 127 mm (5.0 in.) and the semi-minor axes were varied such that elliptical cylinders with aspects ratios of 0.70, 0.85, and 1.00 (circular) were produced. The lay-ups studied were: quasi-isotropic, $[+45/-45/0/90]_s$; axially stiff, $[+45/-45/0_2]_s$, and; circumferentially stiff, $[+45/-45/90_2]_s$. All specimens were cut to the same length, giving a length-to radius ratio of 2.9 for the circular cylinders. Buckling loads were predicted using a simplified estimate based on circular cylinders, and using a STAGS finite-element analysis. Finite-element analysis based on STAGS were also used to study the influence of measured imperfections on the prebuckling and buckling behavior. Measured buckling loads were compared with the predictions from the simple estimate, the finite-element results for the geometrically perfect cylinders, and the finite-elements results for the geometrically imperfect cylinders. Postbuckling and failure characteristics during the testing were also observed. The work was supported, in part, by a grant from the NASA-Langley Research Center and Dr. James H. Starnes, Jr. was the grant monitor. Related work on elliptical cross-section cylinders is reported in the reference below.

Meyers, C.A. and M.W. Hyer, 'Response of elliptical composite cylinders to internal pressure loading,' *Mechanics of Composite Materials and Structures*, vol. 4, no. 4, pp. 317-343, 1997.

Prediction of Compressive Strength of Multi-Directional Composites

Shu, J.Y.
Lawrence Livermore National Laboratory, USA

The compressive strength is a design-limiting parameter of aligned, continuous fiber composite materials. In this paper, the compressive strength of a $0^\circ/90^\circ$ multi-directional laminate is predicted using the finite element method. The compressive failure mechanism is assumed to be microbuckling of the 0°-plies and the delamination between the 0° and 90° plies. The 0°-plies are treated as a homogenized anisotropic couple stress theory solid. The couple stress theory takes into account the effects of fiber bending stiffness and has the fiber diameter as a constitutive length scale. The 90°-plies are modeled by conventional plasticity theory. The interaction between the plies is through a non-linear spring law which allows breaking-of-bond to mimic delamination between the plies. Using the model, the maximum load carried by the composite is calculated. As expected, the bonding between the plies strongly affect the compressive strength. Systematic parametric studies are also carried out with regard to the various geometrical scales (the thickness of the plies and the initial imperfection zone size). The thickness of the 0°-

plies is found to be critical in affecting the compressive strength.

Compression Failure in Graphite Epoxy Composites by Kink Band Formation : A Study Based on Random Breaks Causing Kink Band Initiation

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Drexel University, USA and
Schadler, L.S.
Rensselaer Polytechnic Institute, USA

Kink Band formation is an important mechanism for compressive failure in graphite epoxy composites. Most of the work on this subject focuses on fiber misalignment as the starting point of kink band formation. The misalignment is assumed to cause fiber microbuckling and propagate as an instability in the matrix. The models currently used are also based on fiber misalignment and the misalignment angle. Our work shows that a random set of breaks can lead to an unsupported column of matrix and cause kink band initiation. A stronger interface with a higher stress concentration factor leads to a damaged region perpendicular to the loading direction which increases the yield stress for the composite and a ductile or a brittle interface with a lower stress concentration factor leads to a damaged region at an angle to the loading direction, which lowers the composite yield stress. Our model incorporates the stress concentration factor for the different interfaces to account for the interface property in kink band formation and the results from the model agree well with experimental results.

A Model for Through-the-Thickness Effects in Compression Failure of Fiber Composites

Swanson, S.R.
University of Utah, USA

The compressive strength of many fiber composite materials is lower than the tensile strength, and has been studied extensively in recent years. While there are differences in behavior between the various types of fibers, e.g. aramid fibers are inherently weak in compression, Deteresa has shown that for many carbon and glass fiber types the inherent compressive strength of the fiber can actually be higher than the tensile strength, but this strength is not realized in realistic lamina or laminates. The reasons for this appear to be defects in the fiber straightness and placement. The compressive strength of fiber composites is often considered to be a unique material property, but there is evidence that indicates that it is an "in-situ" property that depends on the details of the laminate layup and test procedure. Examples of this are the very high compressive strength reported by Whitney et al. using axially loaded sandwich columns, bend tests results reported by Wisnom and Jackson, and tests of laminates reported by Hahn et al. and Swanson et al. The above are examples that indicate that the compressive strength of a given fiber and matrix can vary from one test or specimen to another. It is believed by the present author that at least part of this variability is systematic, and can be attributed to through-the-thickness effects. The basic mechanism is that the deformation of fibers with initially wavy paths is supported by the matrix through shear stresses between the fiber and matrix, and that additional shear stress is created by the through-the-thickness variation of the fiber deformation. This through-the-thickness variation depends on the particular layup and test configuration. Examples are adjacent layers such as in the sandwich column tests and tests of laminates with angle plies adjacent to the axial plies, and bend tests. Each of these situations produces through-the-thickness variation of the fiber deformation. A model is presented that gives insight into the effects of this variation. A three dimensional problem of fiber deformation is solved approximately by using Ritz procedure, using a product of displacement functions. These displacement functions each give an exact elasticity solution to an idealized problem in 2 dimensions. The in-plane deformation utilizes the solution of Zhang and Latour, while the through-the-thickness deformation solution is new. Results are given that illustrate the importance of these effects. High compressive strength is predicted for axial sandwich column tests, in good agreement with experiments. The model also predicts that the apparent compressive strength of carbon fiber composites in bend tests can exceed the tensile strength, as observed in experiments.

A Geometrically Nonlinear Analysis of Compressively Loaded Prismatic Plate Structures Using a Reduced Basis Method

Ragon, S.A. and Gürdal, Z.
Virginia Tech University, USA

A geometrically nonlinear analysis capability for the static response of compressively loaded prismatic plate structures is developed. The analysis is based on the nonlinear finite strip method and is applicable for structures, such as stiffened panels or box columns, that can be modeled as assemblages of finite length plate strips. A reduced basis technique as described in [1] is used in conjunction with the finite strip method.

The finite strip analysis is of the semi-analytical multi-term type. Displacement fields are approximated in the longitudinal direction using a series of trigonometric functions, which are chosen so as to make it possible to enforce compatibility between component plates where they meet at an angle. In the transverse direction, both in-plane and out-of-plane displacement fields are approximated using cubic polynomials. Individual finite strips are modeled as

balanced, symmetric laminates, and the resulting structure is loaded by uniform end shortening. Because of the assumed forms of the displacement fields, the boundary conditions at the loaded ends are simply supported out-of-plane. A variety of in-plane and out-of-plane boundary conditions may be simulated at the unloaded edges.

The Principle of Minimum Potential Energy is used to obtain a set of nonlinear algebraic finite strip equations. Instead of solving this (potentially large) set of system equations directly, a reduced basis method is utilized. The finite strip solution vector, x_j, is expressed using a small set of r basis vectors which are the successive derivatives of the finite strip solution vector with respect to the loading parameter, l:. The resulting reduced system equations (of dimension r) are solved using a Newton-Raphson incremental/iterative arc length solution procedure. After each arc-length increment of the solution procedure, the residual vector, Ri, is formed for the full finite strip analysis. A weighted norm of Ri is used to determine whether it becomes necessary to generate a new set of basis vectors. If the norm is greater than a user specified tolerance, , a new set of basis vectors is generated before proceeding with the solution procedure; otherwise, the reduced solution procedure continues with the current set of basis vectors.

Results obtained using the reduced basis/finite strip analysis will be presented for compressively loaded flat plates and blade-stiffened panels. Comparison of results obtained using both the "full" finite strip analysis and the reduced basis techniques will be made. It will be shown that accurate results may be obtained with the reduced solution technique with a greatly reduced number of factorizations of the full finite strip equations.

[1] Noor, Ahmed K., "Recent Advances in Reduction Methods for Nonlinear Problems", Computers and Structures, Vol. 13, pp. 31-44, 1981.

Session: E2-4 Room: Cascade 125 **Time:** T9:30a-11:30a
Chairs: *S. R. Swanson (U. Utah) & J. Y. Shu (LLNL)*

Kink Formation and Growth in Fiber-Reinforced Composites

Nemat-Nasser, S. and McGee, J.
University of California at San Diego, USA

The compression-induced failure mode of polymeric composites changes if the composite is dynamically deformed in the presence of confinement. The confinement promotes localized microcracking leading to the formation of kinks. We have used a 3-inch Hopkinson bar to develop a technique for investigating the initiation and growth of such kinks in S2 fiber-reinforced composites with and without stitch. Preliminary tests were performed in order to develop a method for confinement which does not introduce additional loads on the specimen. The lecture will summarize the results of a set of experiments which have been designed to provide information on the initiation and growth of kink bands. Preliminary results will also be presented on a micromechanical model which is developed to analyze this phenomenon.

Failure Mode Transition in Composites Under Multiaxial Compression

Oguni, K., and Ravichandran, G.
California Institute of Technology, USA

A detailed experimental investigation has been performed on a glass/polyester unidirectional composite over a wide range of multi-axial compressive stress states. The specimen is loaded axially using a servo-hydraulic material testing system and confined laterally by a thick walled cylinder. An acoustic emission (AE) sensor is used to assess the evolution of damage during loading. Post-test microscopy (optical and scanning electron) is used to identify the nature of damage and the failure modes. The measurements are used to construct a failure envelope for glass/polyester composite under multiaxial compression. The results indicate that the compressive (peak) strength of the composite increases with increasing levels of confinement. The failure mode that is observed in an unconfined specimen is axial splitting followed by fiber kink band formation. With confinement, the failure mode changed from axial splitting to kink band formation in the composite.

Micromechanics based models have been developed to explain the failure mode transition and the observed trend in compressive strength. The two observed mechanisms contributing to the failure mode under multi-axial loading are modeled individually. An energy-based model together with a failure criterion is used to simulate axial splitting. Another model, which uses the solution of elastic buckling of a beam on an elastic foundation, is used to simulate kink-band formation under multi-axial loading. For a given lateral confinement, the compressive strength can then be computed as a function of the effective properties of the unsplit and the split composite as well as the fracture energy. An elastic column supported by an elastic foundation subjected to end loads is used to simulate the formation of observed instability, i.e., kink-band formation. The resulting solution shows an increase in compressive strength with increasing lateral confinement as observed experimentally. The splitting and buckling solutions are able to capture the essential features of available experimental data for unidirectional fiber reinforced composites.

High Strain Rate Compression of Fiber Composites

Slaughter, W.S.
University of Pittsburgh, USA

A model is presented for the dynamic compressive behavior of fiber composites under prescribed axial strain rate. The model includes the effects of fiber misalignment and material nonlinearity. A couple stress is used to take into account the fiber bending resistance. An examination of the dynamic axial stress-strain relation shows that the model is consistent with experimental results. For a given strain rate, the axial stress goes through a maximum associated with microbuckling (i.e. the formation of kink bands). The dependence of this dynamic compressive strength on strain rate is also consistent with experiments. Finally, the model is used to predict the kink band width as a function of the strain rate; at high axial strain rates, the kink band width is about one-half that for quasi-static loading.

Scaling of Tensile and Compressive Brittle Failures of Fiber Composites

Bažant, Z.P. and Becq-Giraudon, E.
Northwestern University, USA

Similitude and scaling are the most fundamental aspects of every physical theory. In mechanics of solids, however, little attention has been paid to the scaling of failure and until about a decade ago it has been generally assumed that the observed size effect on nominal strength of structures must always be explained by Weibull-type randomness of strength. Detailed analysis shows, however, that this scaling theory does not capture the main cause of size effect in nonlinear fracture mechanics, observed in quasibrittle materials, including fiber-polymer composites as well as concrete, ice, rocks, and various toughened ceramics which exhibit a large fracture process zone and allow stable growth of large cracks prior to failure. Rather, the dominant source of size effect appears to be deterministic and consists in the release of stored energy.

In the present paper, the effect of structure size on the nominal strength of unidirectional fiber-polymer composites, failing by propagation of a kink band with fiber microbuckling, is analyzed experimentally and theoretically. Tests of novel geometrically similar carbon—PEEK specimens, with notches slanted so as to lead to a pure kink band (without shear or splitting cracks), are conducted. They reveal the existence of a strong (deterministic, non-statistical) size effect. The doubly logarithmic plot of the nominal strength (load divided by size and thickness) versus the characteristic size agrees with the approximate size effect law proposed for quasibrittle failures in 1983 by \B\. This law represents a gradual transition from a horizontal asymptote, representing the case of no size effect (characteristic of plasticity or strength criteria), to an asymptote of slope -1/2 (characteristic of linear elastic fracture mechanics, LEFM). A new derivation of this law by J-integral analysis of energy release is given. The law is further generalized to notch-free specimens attaining the maximum load after a stable long kink band growth. The nominal strength of specimens failing at the initiation of a kink band from a smooth surface is predicted to also exhibit a (deterministic) size effect. A different size effect formula is derived for this case by analyzing the stress redistribution, and is shown to approximately agree with recent test results reported by Fleck for the effect of the size of a hole. The size effect law for notched specimens permits easy identification of the fracture energy of the kink band and the length of the fracture process zone at the front of the band solely from the measurements of maximum loads. The results suggest that the current design practice, which relies on the strength criteria (or plasticity) and thus inevitably misses the size effect, is acceptable only for small structural parts and, in the interest of safety, should be revised in the case of large structural parts.

Crack Interaction Problems in a Fiber-Matrix Composite: Debonding and Broken Fiber

Demir, I., King Saud University, Saudi Arabia

Understanding the behavior of micro-imperfections around fibers and matrix is important in analyzing the global response of the composite materials. Although there have been numerous studies on cylindrical cracks at the fiber matrix interfaces to model the debonding process, a complete analysis of the interaction of such cracks among themselves and with other types of imperfections such as broken fibers, annular matrix cracks or fiber tips has not been fully investigated yet.

This paper is an attempt to model interaction problem between numerous fiber matrix debondings (cylindrical interface cracks) and the broken fibers or annular cracks. The solution is based on the dislocation density distribution modeling of cracks. Since the rotational shapes involved in the problem special dislocation loops have been used to model these type of problems. They can be classified basically as Volterra and Somigliana types of dislocations. A Somigliana type of interface ring dislocation is capable of modeling interfacial debonding around a fiber and Volterra type (circular prismatic loop) is capable of modeling both another mode of the same debonding and broken fiber (penny shaped crack terminating at the interface) as well as annular matrix or fiber cracks. Basic solutions for the above dislocation loops are restricted to the axisymmetric case and the present solution considers the multiple coaxial cracks where axisymmetry is preserved and the external loads which

are capable of creating all three modes are applied accordingly.

The solution process considers all the unknown dislocation density distributions at once either along the axial or radial directions This coupled solution results a set of coupled Cauchy singular integral equations of the second kind where the distribution of the Somigliana or Volterra dislocations along each cracks are the unknown functions to be found. The means of handling non-axisymmetric cases have also been discussed.

Symposium E3
Topics in Theoretical and Applied Elasticity
Organizers
Y.C. Chen
University of Houston, USA
&
D. Steigmann
University of California at Berkeley, USA

Session: E3-1 Room: Cascade 125 **Time:** M10:00a-12:00p
Chairs: *C. Ru (U. Alberta) & P. Schiavone (U. Alberta)*

Saint-Venant Decay Rates for an Isotropic Inhomogeneous Linearly Elastic Solid in Anti-Plane Shear

Horgan, C.O.
University of Virginia, USA

The purpose of this research (joint work with M.R., Scalpato [1]) is to investigate the effects of material inhomogeneity on the decay of Saint-Venant end effects in linear isotropic elasticity. This question is addressed within the context of anti-plane shear deformations of an inhomogeneous isotropic elastic solid. The mathematical issues involve the effects of spatial inhomogeneity on the decay rates of solutions to Dirichlet or Neumann boundary – value problems for a second – order linear elliptic partial differential equation with variable coefficients on a semi – infinite strip. The elastic coefficients are assumed to be smooth functions of the transverse coordinate. The estimated rate of exponential decay with distance from the loaded end (a lower bound for the exact rate of decay) is characterized in terms of the smallest positive eigenvalue of a Sturm – Liouville problem with variable coefficients. Analytic lower bounds for this eigenvalue are used to obtain the desired estimated decay rates. Numerical techniques are also employed to assess the accuracy of the analytical results. The results are applicable to continuously inhomogeneous materials and, in particular, to functionally graded materials.

1. M.R. Scalpato and C.O. Horgan, Saint-Venant Decay Rates for an Isotropic Inhomogeneous Linearly Elastic Solid in Anti – Plane Shear, *J. of Elasticity* (1997) (in press).

Saint-Venant's Problem for a Second-Order Elastic Pretwisted Bar Using Signorini's Perturbation Method

dell'Isola, F.
Universita di Roma, Italy, and
Batra, R.C.
Virginia Polytechnic Institute & State University, USA

We use Signorini's expansion to analyze deformations of a straight, prismatic, isotropic, stress free, homogeneous body made of a second-order elastic material and loaded as follows.

It is first twisted by an infinitesimal amount and then loaded by applying surface tractions, with nonzero resultant forces and/or moments, only at its end faces. The centroid of one end face is taken to be rigidly clamped. By using a semi-inverse method, the problem is reduced to that of solving two plane elliptic problems involving six arbitrary constants that characterize flexure, bending, extension, and torsion superimposed upon the infinitesimal twist. It is shown that the Clebsch hypothesis is not valid for this problem.

A second –order Poisson's effect, not of the Saint-Venant type, may also occur in these problems.

The Net Interaction Force Between Two Skew Dislocations in an Elastically Anisotropic Half-Space

Barnett, D.M.
Stanford University, USA

It is generally known that the total interaction force between two non-parallel infinitely long straight dislocations in an infinite isotropic linear elastic medium is independent of their separation. Orlov and Indenbom (1969) have shown that this result is valid for arbitrary elastic anisotropy, and that the net interaction force may be computed explicitly without knowing details of the Stroh solution for the field of a straight dislocation in an infinite anisotropic medium. In the present work it is shown that the independence of the total interaction force on separation remains valid for two skew dislocations in an anisotropic half-space (each dislocation being parallel to the traction-free half-space boundary). If we refer to the dislocation closest to the half-space free boundary as (1) and to the other dislocation as (2), we find the remarkable result that the total interaction force of (1) on (2) vanishes, while the total interaction force of (2) on (1) is precisely twice the total interaction force which (2) exerts on (1) in an infinite medium. The fact that the two net interaction forces are not equal and opposite (unless they both vanish) is due to the lack of translational invariance normal to the boundary of a semi-infinite medium. This set of results is called Nix's Theorem, after W. D. Nix, whose numerical computations for isotropic half-spaces suggested that

the results might be true for half-spaces of arbitrary anisotropy, thus motivating the present proof. The implications of the theorem and the ease with which the interaction forces can be computed should prove useful in the modeling of dislocated thin films.

Integral Equation Methods in Plane-Strain Elasticity with Boundary Reinforcement

Schiavone, P. and Ru, C.Q.
University of Alberta, Canada

We develop a linear theory of elastic boundary reinforcement for plane deformations of elastic solids. The reinforcement consists of a thin elastic coating bonded to part of the boundary of the elastic solid. The elastic properties of the coating incorporate both extensibility and bending rigidity. Interior and exterior mixed boundary value problems are formulated and solved using integral equation methods. The boundary-value problems are reduced to systems of singular integro-differential equations on the coating. Finally, analytical solutions of the boundary value problems are obtained in the form of integral potentials.

Isoperimetric Inequalities for the Stresses due to Inhomogeneities

Wheeler, L.
University of Houston, USA

Inhomogeneities serve as stress concentrators. For an inhomogeneity of given elastic moduli imbedded in a matrix of distinct but also given moduli, the nature of the stress concentration is determined by the shape of the inhomogeneity. If the concentration of the stress is measured by greatest principal stress, is there a shape which minimizes the stress concentration? Under mil and reasonable assumptions on the material properties and the applied loading, the answer is affirmative and in these cases, an isoperimetric inequality results. The associated optimum shape is a suitably proportioned ellipsoid. In this presentation we present an indirect derivation of the associated isoperimetric inequalities.

Session: E3-2 Room: Cascade 125 **Time:** M1:30p-3:30p
Chair: *P. Rosakis (Cornell)*

Fluid Capillarity with Curvature-Dependent Elasticity

Steigmann, D.
University of California, Berkeley, USA

A theory for fluid capillarity incorporating local curvature in the free energy function is developed. Fluid films are regarded as elastic surfaces with a free energy that is insensitive to certain unimodular transformations. This is shown to yield a constitutive dependence on the Gaussian curvature of the surface but not on the mean curvature, in contrast to alternative theories that purport to describe fluid-like responses. Necessary conditions for energy minimizers are discussed and used to motivate a phenomenological model for the emergence of certain 'biocontinuous' phases in microemulsions.

A Simple, Logical, Comprehensive Approach to Nonlinear Shell Theory

Simmonds, J.G.
University of Virginia, USA

There is much confusion in both the engineering and mathematical literature concerning shell theory for at least six reasons.

1. The misinterpretation and misapplication of the Kirchhoff hypothesis.
2. A failure to appreciate what parts of shell theory are exact and what parts are necessarily approximate.
3. The introduction of assumptions that are, at once, too elaborate and too restrictive.
4. The failure to properly distinguish between physical and mathematical approximations.
5. The use of forms of the governing equations (poor choice of the dependent variables) which may lead to ill-conditioned numerical solutions or which may not reduce easily to important special cases (e.g., membrane theory, inextensional bending).
6. Overly simplified or overly elaborate thermodynamics.

This talk starts with fundamental laws (``axioms") of (thermo-)continuum mechanics written in integral-impulse form. Thus, such phenomena as shocks and concentrated loads can be handled in a simple, natural way. Specialized to shell-like bodies, these equations yield, automatically and *without approximation,* definitions of stress resultants, stress couples, an entropy resultant, a deformed position vector, a spin, and a rotary inertia tensor, all defined over a *surface of mass* (analogous to the center of gravity of classical mechanics) which, in general, is *not* the midsurface of the shell and which , in general, does *not* consist of the same material particles as the shell deforms. Smoothness implies simple vector equations of motion and these, in turn, lead to a mathematical power identity is, in fact, a statement of conservation of physical energy. A *thermoelastic* shell is one that possesses a stored (free-) energy function (which, as in 3-dimensional nonlinear elasticity, *must* ultimately come from experiments). Thus, not only can *all* approximations in shell theory be thrown into that part which is intrinsically empirical, but the "Kirchhoff Hypothesis" can now be interpreted, not as an unjustified *a priori* kinematical constraint, but as the assumption that the stored energy of a shell does not depend on the shear-rotation strain. Finally, it is shown that a Legendre-Fenchel transformation can often lead to an especially symmetric and well-conditioned form of the full set of governing equations.

Extensional Oscillations and Waves in Elastic Rods which Account for Thickness-Stretch Effects

Krishnaswamy, S.
University of Nebraska-Lincoln, USA

We study the dispersive nature of propagating extensional waves in an infinitely long elastic rod within the framework of the linear theory of a Cosserat rod with two directors. We identify certain material constants in the theory in a manner that is different from those used by others, and consequently show that the resulting theory better captures the high-frequency dynamical behavior of three-dimensional rod-like bodies. This high-frequency behavior can be modelled well within our theory because we explicitly account for lateral deformation in the rod.

Extremum Principles for Nonlinearly Elastic Membrane Problems

Ogden, R.W.
University of Glasgow, Scotland, and
Haddow, J.B.
University of Victoria, Canada

In this paper the validity of minimum and maximum complementary energy principles for certain (incompressible or compressible) isotropic elastic membrane problems is established for tensile states of membrane stress. This is based on the assumption that the strain energy is strictly convex as a function of the two independent (in-surface) stretches, an assumption which is verified for specific forms of stain energy. The stronger condition of strict convexity as a function of the in-surface deformation gradient imposes the additional requirement that the principal stresses be tensile. Upper and lower bounds on the actual energy are then obtained using appropriate choices of admissible stress and deformation fields.

The theory is illustrated by application to the axially symmetric extension of an initially circular cylindrical membrane whose end radii remain fixed during deformation. It is found that, for the particular forms of strain energy used, the upper and lower bounds are remarkably close and a very good estimate of the actual energy is therefore obtained; this is demonstrated by numerical calculations. The associated deformed geometry of the membrane surface is also calculated from both the upper and lower bounds and again the results are seen to be very close. The numerical results also confirm the required positiveness of the principal membrane stresses.

On Calculation of Interfacial Stresses in Film-Substrate Systems

Ru, C.Q.
University of Alberta, Canada

Thermal mismatch induced stresses are a common cause of failure of many film-substrate systems such as thermal barrier coating and microelectronic packaging. Classical methods are primarily focused on calculation of thermal stresses in film and the change in the curvature of film-substrate system. However, it is the interfacial stresses that are responsible for the integrity of the film-substrate system. Hence, more recently, considerable effort has been devoted to calculation of thermal-mismatch induced interfacial stresses in film-substrate systems. Since a knowledge of interfacial stresses is often just a prerequisite for more complicated analysis of failure of the film-substrate system, of particular interest is easy-to-use formulas with sufficient accuracy that avoid complicated three-dimensional stress analysis. To this end, an interesting approach based on theory of strength of materials has been developed by E. Suhir (1986-1997). Remarkably, two simple linear ordinary differential equations have been derived by Suhir for determination of the interfacial shearing and peeling stresses in a one-dimensional bilayer beam. The present work aims to extend Suhir's method to more general two-dimensional film-substrate multilayer system. In doing so, two partial differential equation governing the interfacial stresses are derived for each interface of the multilayer system. Detailed discussion is given for a three-layer film-substrate system. Interfacial stresses calculated using this method are compared to more accurate numerical solutions and experimental results and the accuracy of the present method is evaluated.

Session: E3-3 Room: Cascade 125 **Time:** M4:00p-6:00p
Chair: *S. Krishnaswamy (Nebraska-Lincoln)*

Natural Strain Invariants for Isotropic Finite Hyperelasticity

Criscione, J.C.
Johns Hopkins University, USA
Humphrey, J.D.
Texas A&M University, USA, and
Hunter, W.C.
Johns Hopkins University, USA

We propose a new set of coordinate-invariant scalar measures of a symmetric tensor that are completely independent: one is the trace, another is the deviatoric magnitude, and the third is the deviatoric mode. We consider them completely independent because if two are fixed the third can assume all realistic values (i.e. unconstrained). These invariants are particularly useful for a natural strain description because $\eta \equiv \ln \mathbf{U}$ (or $\ln \mathbf{V}$) additively decouples into

dilatational (spherical) and distortional (deviatoric) parts. We thus define

$$K_1 = tr(\eta) = \ln(J),$$

$$K_2 = \sqrt{(\eta - \tfrac{1}{3}K_1\mathbf{I}):(\eta - \tfrac{1}{3}K_1\mathbf{I})},$$

$$K_3 = 3\sqrt{6}\det\left(\frac{\eta - \tfrac{1}{3}K_1\mathbf{I}}{K_2}\right),$$

wherein $J \equiv \det(\mathbf{F})$ and $():()$ is the tensor contraction. Hence, K_1, K_2, and K_3 respectively measure: volumetric strain, distortion magnitude, and distortion mode. Note that the mode is a normalized index, $K_3 \in [-1,1]$, that describes any pattern of distortion. For example, consider a body undergoing infinitesimal (K_2 small) or finite (K_2 large) distortion: $K_3=1$ for uniaxial extension, $K_3=0$ for pure shear, and $K_3=-1$ for uniaxial contraction. Furthermore, $\partial K_1/\partial\eta$, $\partial K_2/\partial\eta$, and $\partial K_3/\partial\eta$ are kinematic tensors orthogonally-related to each other (note: **A** and **B** are orthogonally-related tensors if $\mathbf{A}:\mathbf{B}=0$). We thus assert that these K_i form an *orthogonal invariant set*, and we use the fact that only one depends on dilatation to state that they admit *dilatational separability*. Assuming $W(K_1,K_2,K_3)$, the Cauchy or true stress decomposes into three orthogonally-related stress tensors, each with physical significance: *baric stress* (pressure-like and collinear with the dilatation strain $\frac{1}{3}K_1\mathbf{I}$), *co-abaric stress* ("shear" collinear with the distortion strain $\eta-\frac{1}{3}K_1\mathbf{I}$), and *con-abaric stress* ("shear" orthogonal or contrary to both $\frac{1}{3}K_1\mathbf{I}$ and $\eta-\frac{1}{3}K_1\mathbf{I}$). Using this terminology we may state that the K_1 response term gives the baric stress, the K_2 response term gives the co-abaric stress, and the K_3 response term gives the con-abaric stress. Moreover, in general, W admits a reduced form of separable and testable terms. The utility of these invariants allows us to formulate a form of W for rubber that describes the biaxial stretch data of both Rivlin and Saunders (1951) and Jones and Treloar (1975) with good accuracy.

On the Existence of a Stretch for a Prescribed Stress in Isotropic, Incompressible Elastic Materials

Nordenholz, T.R. and O'Reilly, O.M.
University of California at Berkeley, USA

In this talk we shall show that an isotropic, incompressible elastic material can support any system of homogeneous tractions if it satisfies a strengthened form of Truesdell's inequalities. Specifically, if this strengthened condition is satisfied, then the Cauchy and first Piola-Kirchhoff stress tensor can assume all values. These results extend Rivlin's existence results for certain Neo-Hookean and Mooney-Rivlin's materials. The strengthened condition implies the Baker-Ericksen inequalities and we will show how these imply a restriction due to Carroll and McCarthy. It also implies two growth conditions either one of which is sufficient to guarantee the existence result for the Cauchy stress tensor.

The Inverse Convexity Condition and its Implications in Nonlinear Elasticity

Rosakis, P.
Cornell University, USA

We consider an alternative constitutive inequality of convexity type for nonlinear elastostatics of unconstrained materials. This inequality does not suffer from the drawbacks of strict convexity of the stored energy function. It ensures uniqueness for the displacement problem but does not preclude buckling. It is consistent with frame indifference and allows the stored energy to grow unbounded as the Jacobian determinant of the deformation goes to zero. We discuss some of the implications of the inequality on mechanical behavior and uniqueness of classical solutions to the displacement boundary value problem. We also show that it predicts nonexistence of solutions for sufficiently severe loading in certain problems. The implications of this on mechanical failure are examined.

New Existence Results in Nonlinear Elastostatics via Global Continuation Methods

Healey, T.
Cornell University, USA

We begin with a discussion on the physical requirements of nonlinear elasticity (e.g., injectivity, growth conditions and traction boundary conditions) that preclude a standard global analysis via the method of Leray and Schauder in 3d nonlinear elastostatics. We then discuss some recent generalizations of the Leray-Schauder approach yielding detailed global existence of classical solutions to broad classes of boundary-value problems in nonlinear elastostatics.

On the Application of Covariance to Anisotropic Finite Elasticity

Papadopoulos, P. and Lu, J.
University of California, Berkeley, USA

The postulate of covariance (understood here as invariance under superposed diffeomorphisms) has important theoretical and computational implications in non-linear elasticity. In particular, the covariant statement of energy balance is equivalent to local statements of the balance laws [1] and gives rise to the classical Doyle-Ericksen stress formula for Green-elastic materials. Computationally, covariance allows for the direct derivation of the stress response and elasticity tensor in terms of the Cauchy stress tensor, therefore furnishing a suitable basis for Eulerian finite element formulations.

Starting from a strain energy function W=W(**F**,**G**,**g**), where **F** is the deformation gradient, **G** is a referential metric and **g** is a spatial metric, it can be easily established that covariance of W implies isotropy [1]. This work examines the role of covariance in anisotropic elasticity. To this end, anisotropy is embedded to the strain energy function by admitting the existence of structural tensors and appealing to the relevant representation theorems [2,3]. It is shown that the postulate of covariance is applicable and consistent with the assumed material symmetries. In addition, covariance results in a natural derivation of the constitutive equations for anisotropic Green-elastic materials.

1. J.E. Marsden and T.J.R. Hughes. *Mathematical Foundations of Elasticity*, Prentice-Hall, Englewood Cliffs, 1983.
2. J.-P. Boehler. A Simple Derivation of Representations for Non-Polynomial Constitutive Equations in Some Cases of Anisotropy. *Zeit. Angew. Mat. Mec.*, 59:157-167, 1979.
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Session: E3-4 Room: Cascade 125 **Time:** T1:00p-3:00p
Chairs: *D. P. Warne (U. Tennessee) & P. G. Warne (Maryville College)*

Boundary Layer Solutions in Elastic Solids

Chen, Y.C.,
University of Houston, USA and
Rajagopal, K.R.
Texas A & M University, USA

Whether it is the motion of fluids or solids, most of the interesting phenomena often take place adjacent to solid boundaries or at interfaces. Prescribing boundary conditions and describing the observed phenomena adjacent to boundaries remain the most challenging aspect of mechanics, especially when non-linear materials are concerned. By a boundary layer in solids, we mean a narrow region adjacent to a boundary wherein the strains are large and the full non-linear equations are assumed to hold, while exterior to this region the strains are small and the linearized equations are expected to hold. The thickness of the boundary layer can be chosen so that a large portion of the strain is confined in boundary layer. It is also possible to define boundary layers based on stresses.

Circumferential shear deformation in an annular domain is studied for a large class of incompressible isotropic elastic materials. It is demonstrated that large strains are confined in a region adjacent to a boundary. The size of this region is quantified. An approximate solution technique for the deformation of non-linear elastic solids is studied. In this solution, akin to the boundary layer approximation in classical fluid mechanics, the full non-linear problem is solved in a relatively small region of large strain, while the linearized problem is solved in the remaining region. Error estimates for the approximate solution are obtained.

An Outer and Inner Tensor Product

Warne, P.G.
Maryville College, USA

An extended tensor dot product is proposed with a view toward direct notation manipulations among tensors of various ranks. The advantages of this extension lie in that it allows, in conjunction with the dyadic product a way to move easily through dimensions, and also allows for representations in direct notation of physical relationships and quantities previously limited to indicial notation. This product gives a physical meaning to, and direct representation of, the alternator tensor, and retains the geometrical flavor often lost with indicial representations When viewed within the existing framework, this product is consistent with known results and also provides a relationship between indicial notation and many algebras both previously and currently being developed (e.g. D. Hestenes' geometric algebra and W. Hamilton's quaternions).

Plane Deformations in Incompressible Nonlinear Elasticity

Warne, D.P.
University of Tennessee, USA, and
Warne, P.G.
Maryville College, USA

Much of what is known concerning problems within the nonlinear theory of elasticity has followed from symmetry assumptions such as radial or axi-symmetry on the deformation field, and the associated analysis involves systems of nonlinear ordinary differential equations. Inherent in all such studies is the question of what, if anything, lies beyond the assumed form of the deformation field. Relaxing such restrictions on the deformation results in highly complicated systems of nonlinear partial differential equations. We consider here a very general class of (non-symmetric) plane deformations in incompressible nonlinear elasticity. Analysis to determine the types of deformations possible, that is, solutions of the governing systems of nonlinear partial differential equations and constraint of incompressibility, is developed in general. The Mooney-Rivlin material model is then considered as an example, and a new solution to the governing equations is found. The novel approach taken here requires the derivation and use of a material formulation of the governing equations; the traditional approach employing a spatial formulation in which the governing equations hold an unknown region of space is not conducive to the study of deformation fields containing more than one independent variable.

Pure Bending of Incompressible Elastic Plates

Haughton, D.M.
University of Glasgow, Scotland

We consider the bifurcation problem for three dimensional isotropic, incompressible, non-linearly elastic plate subjected to an axial compression and a pure bending in the plane.

The aims of the work are two-fold. Firstly to get some basic information about plates and bars in flexure which may help when dealing with more complicated geometries, for example the flexure of tubes. Secondly to investigate the interaction of the barrelling/buckling modes for a plate under compression with the bifurcation modes due to the flexure. We see how bending the plate stabilizes it with respect to axial load.

Instability of an Internally Constrained Hyperelastic Material

Beatty, M.
University of Nebraska-Lincoln, USA, and
Pan, F.
Cornell University, USA

The wave speed criterion [1-2] is applied to discuss restrictions on the material response functions of an isotropic, Bell constrained material in order that small amplitude, plane waves may propagate in the material with real wave speeds. The case of a body subjected to a biaxial stress is related to the elastic stability of a Bell constrained slab. We show that two cases among five reported in [3] for the elastic stability of a thick plate cannot support such waves; and hence, as remarked in [3], these cases are not possible and must be excluded. The question of the stability of the equibiaxial deformations of a Bell constrained material under an all-around Cauchy stress, suggested by Beatty and Hayes [4], is investigated. It is shown that for a general Bell material model, the state of equibiaxial deformation under an all-around Cauchy stress is materially unstable, unless all stretches are equal to one, their value I the initial undistorted state.

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Session: E3-5 **Room:** Cascade 125 **Time:** T3:30p-5:30p
Chair: *Y. C. Chen (U. Houston)*

A Model for Nonlinear Viscoelastic Single Mode Response of an Elastomeric Bushing

Wineman, A., VanDyke, T., Shi, S. and Lee, S.B.
University of Michigan, Ann Arbor, USA

An elastomeric bushing is a device used in automotive suspension systems to cushion the force transmitted from the wheel to the frame of the vehicle. A bushing is essentially an elastomeric hollow cylinder which is bonded to a solid metal shaft at its inner surface and a metal sleeve at its outer surface. The shaft is connected to the suspension and the sleeve is connected to the frame. The elastomeric cylinder provide the cushion when it deforms due to relative motion between the shaft and sleeve. The relation between the force applied to the shaft or sleeve and their relative deformation is nonlinear and exhibits viscoelastic properties.

A force-displacement relation for the bushing plays an important role in determining the dynamical response of the suspension system. This work presents a proposed relation for single mode response of the bushing assembly. The force is given by a single integral constitutive equation which is nonlinear in the displacement history, accounts for viscoelasticity and is also computationally convenient for use in multi-body dynamics analysis. It depends on a force relaxation function, the bushing property in the model. An experimental method for determining this property is outlined and results of its application are presented. Forces due to various prescribed displacement histories computed from the model are in good agreement with experimentally determined forces.

A boundary value problem for single mode bushing response is formulated in which the nonlinear viscoelastic elastomeric material is described by a constitutive equation developed elsewhere from experimental data. The boundary value problem represents the exact force-displacement relation, but it is an implicit relation and requires extensive computation time to implement. Numerical solutions of the boundary value problem provide data which are used in the method for determining the force relaxation function in the proposed explicit force-displacement relations. Numerical predictions carried out with the proposed model and the exact model are in close agreement. The proposed force-displacement relation can thus be regarded as a useful approximation to the exact one.

'Springback' and Related Effects in Composites Forming

Spencer, A.J.M.
University of Nottingham, England

Curved shells of fibre-reinforced thermoplastic composite materials are often formed by pressing stacks of sheets of initially flat, unidirectionally reinforced, but differently oriented, thermoplastic material into a mould at a high temperature. At the forming temperature the material is effectively fluid, although its deformation is constrained by the presence of the fibres. On cooling, solidification, and removal from the mould, the product is usually found to have distorted from the shape of the mould. This distortion is due to thermoplastic deformation that accompanies cooling. Since the solid composite materials strongly anisotropic the amount of thermal contraction depends strongly on direction in the material, which results in a change of shape as well as a uniform contraction on cooling. It is clearly desirable to have a capability to design the mould so as to achieve the desired final shape. For channel sections (shells with single curvature) there exists a very simple thermoelastic analysis for slow cooling of orthotropic sections, which determines a stress-free distorted final configuration. In practice this analysis has been found to give good results not only for slow cooling and elastic response but also for rapid cooling and for viscoelastic material behavior. Here it is shown that the thermoelastic analysis can be extended to a large class of thermoviscoelastic materials, and that he results are virtually unchanged by this extension. We also discuss the effect of rapid cooling, in which case a solidification front progresses through the material, and it is necessary to take account of through-thickness temperature gradients. For rapid cooling it is also found that the direction as well as the rate of cooling has a significant effect.

On Finitely Deforming Elastic-Viscoplastic Materials

Casey, J. and Nath, D.S.
University of California, Berkeley, USA

A purely mechanical theory is presented for describing the behavior of materials having a rate-independent elastic response but a rate-dependent plastic response. The theory, which evolved out of work by Naghdi and co-authors on rate-independent and rate-dependent solids, is formulated in Lagrangian strain-space, is of rate-type, and accommodates arbitrary motions of the continuum. A prescription is given for the identification of plastic strain. The use of dynamic yield surfaces" in stress-space, a common feature in existing theories, is found to be unnecessary. Several special types of response, including the rigid-viscoplastic case, are discussed.

Inflation of an Elastomer Cylinder which Exhibits Stress Softening Residual Deformation

Haddow, J.B. and Wegner, J. L.
University of Victoria, Canada

The Mullins effect [1], also known as stress softening, refers to a decrease in the elastic moduli of certain elastomers, due to prior deformation. Elastomers which exhibit the Mullins effect usually exhibit residual deformation when unloaded from a state of homogeneous finite deformation. The objective of this paper is to consider the finite plane strain deformation of a thick walled cylindrical tube composed of an elastomer which exhibits stress softening and residual deformation. A material model for homogeneous plane strain deformation with one principal stress equal to zero is proposed. This model assumes incompressibility and is based on the neo-Hookean stress-stretch relation. It is also assumed that a superimposed hydrostatic stress does not influence the plane strain of loading and unloading from the virgin state of the tube is considered and numerical results, for the residual stress distribution and the relation between internal pressure and inside radius, are presented for a particular set of parameters.

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A Model for Nonlinear Viscoelastic Coupled Mode Response of an Elastomeric Bushing

Wineman, A. and Lee, S.B.
University of Michigan, Ann Arbor, USA

An elastomeric bushing is a device used in automotive suspension systems to cushion the loads transmitted from the wheel to the frame of the vehicle. A bushing is essentially an elastomeric hollow cylinder which is bonded to a solid metal shaft at its inner surface and a metal sleeve at its outer surface. The shaft is connected to the suspension and the sleeve is connected to the frame. The elastomeric cylinder provides the cushion when it deforms due to relative motion between the shaft and sleeve. The relation between the force or moment applied to the shaft or sleeve and the relative displacements or rotations is nonlinear and exhibits features of viscoelasticity.

A boundary value problem is formulated for the coupled axial and torsional mode response of a bushing, in which the nonlinear viscoelastic elastomeric material is described by a constitutive equation developed elsewhere from experimental data. This boundary value problem represents an exact but implicit force-displacement relation which requires extensive computation time to implement and is thus not suitable for use in multi-body dynamics numerical simulations. A second model is proposed in which the axial force and torsional moment are given by single

integral constitutive equations which are nonlinear in the axial displacement and rotation histories, and which account for viscoelasticity. Each equation contains a relaxation function which depends on the axial displacement and rotation. The relaxation functions are constructed using numerical results obtained by solving the boundary value problem. The resultant model is suitable for use in multi-body dynamics numerical simulations. Numerical predictions carried out with the exact model are in very good agreement with those of the proposed model. The proposed force-displacement relation can thus be regarded as a useful approximation to the exact one.

Session: E3-6 Room: Cascade 125 **Time:** W9:30a-11:30a
Chair: *J. Hashemi (Texas Tech)*

A Class of Exact Solutions in Elastic Dielectrics

Chowdhury, K.L.
University of Calgary, Canada

Mindlin's theory of elastic dielectrics {1} assumes dependence of the internal energy density function on the strain tensor, polarization vector and the polarization gradient tensor. This theory yields a system of coupled linear field equations in displacement and polarization vectors and the potential of the Maxwell's field with the constitutive relations between the stress tensor and the polarization vector even for the centrosymmetric isotropic materials. The presence of the polarization gradient terms in the energy density explains observed phenomena, such as the capacitance of thin films, optical and acoustical activity in alpha quartz and the surface energy of deformation and polarization.

Due to the complex nature of the basic system of equations of the Mindlin's theory, very few boundary value have been solved in the frame-work of this theory. Schwartz {2} constructed Pakovitch functions analogous to those of classical elasticity and used these to find fundamental solutions for the problem of a concentrated force in an infinite elastic dielectric continuum. The problem of stress concentration at the surface of cylindrical hole in an infinite dielectric continuum subjected to longitudinal tension has been solved by Gou {3} using the displacement functions earlier constructed by Schwartz {2}.

This paper deals with one-dimensional boundary value problems within the Mindlin's theory of elastic dielectrics with polarization gradient. Exact closed form expressions are obtained for the components of displacement and polarization vectors, the Maxwell's potential field, the stress and electric tensor components and the surface energy of deformation and polarization for the problems of a plate, a cylindrical shell and a spherical shell with one surface stress free and the other subject to (u, P, phi)=(0,0,0). These type of boundary constraints lead to identically zero solutions in other linear theories but in the Mindlin's theory, allowance of such a latitude is inherently due to the presence of the polarization gradient term in the free energy density function. By letting one of the boundaries approach infinity, the displacement and polarization, the potential field and the surface energy deformation and polarization are derived for the half space and for an infinite space with cylindrical and spherical cavities. The surface energy of deformation and polarization in each case depends on the curvature of the free surface and is found to agree with the known results.

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{2} Schwarts, J. Solutions of equations of equilibrium of elastic dielectrics, ibid, 5, 1209 (1969).
{3} Gou, P.F., Effects of gradient of polarization on stress concentration at a cylindrical hole in an elastic dielectric, ibid, 7, 1467 (1971).

A Galerkin Type Solution for Thermo-Microstretch Elastic Media.

De Cicco, S.
Istituto di Costruzioni, Italy

The theory of microstretch elastic solids has been introduced by Eringen [1] to characterize the behavior of some materials with inner structure. For example, composite materials reinforced with chopped elastic fibers, porous media whose pores filled with gas or inviscid liquid, asphalt and other industrial materials such as "solid-liquid" crystals should be characterizable by microstretch solids.

Microstretch materials, roughly speaking, are micropolar materials with an extra independent degree of freedom, including expansions and contractions of the microstructure. Thus, the theory of microstretch continua is a generalization of theory of micropolar continua [2] and can be used as mathematical model for many different materials that fall outside the domain of micropolar elasticity. Microstretch theory is now well-established and it has found many important applications [cf. e.g. 3-6]. The linear dynamic theory of thermo-microstretch elastic solids was presented by Eringen in [7], where he established a uniqueness theorem for the mixed boundary-initial-value problem. Moreover, the theory was illustrated with the solution of one-dimensional dynamical problem. The asymptotic behavior of solutions and an existence result have been presented by Bofill and Quintanilla [8]. The purpose of this paper is to establish a representation of Galerkin type in the framework of the linear dynamic theory of thermo-microstretch elastic solids. Then, we apply this representation to study the problem of concentrated heat source in the case of steady vibrations.

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Reflection of Harmonic Waves at the End of a Cylinder with a General Cross-Section

Taweel H. and Dong, S.B.
University of California, Los Angeles, USA

The reflection phenomenon at the free end of a semi-infinitely long prismatic cylinder due to a steady-state incident wave is investigated. The cross-section of the cylinder may be of arbitrary geometry and composed of any number of perfectly bonded materials, each of which may possess distinct rectilinear anisotropic mechanical properties. The analysis is predicated on linear three-dimensional elasticity.

The governing equations of motion are based finite element modeling of the cross-sectional behavior with the axial dependence and time left undetermined at the outset. In the first step, an eigen analysis is performed to establish all admissible propagating waves and all end modes corresponding to the frequency of the incident wave. Based on these eigenmodes, their corresponding stress eigenvectors are constructed. Then, the traction-free end condition is enforced on an integral basis in accordance with a variational principle. This traction-free end specification leads to a set of equations defining all of the amplitudes of the reflected traveling waves as well as the end modes (i.e., standing vibrations) used in the representation of the reflection phenomenon. An energy balance is carried out as a measure of the precision with respect to the total number of modes used to represent the traction-free end condition.

Examples of (1) isotropic, homogeneous circular rod, (2) isotropic rectangular rod, (3) three-layer ± 30° fiber composite beam and (4) two-layer ± 30° fiber composite beam are given to illustrate the reflection phenomena in these geometries.

Determination of Stresses in Shells of Elliptical Cross-Section Under Internal Pressure

Zheng, Q.S., Hashemi, J., Cárdenas-García, J.F. and Vallabhan, C.G.V.
Texas Tech University, USA

Cargo tank vehicles are responsible for delivery of 79% of the hazardous materials transported by highway in the United States. The majority of these tanks have non-circular cross sections (elliptical, oval). There are currently no analytical methods available to determine the stresses in the shells and heads of non-circular cross section tanks. Basic methods must be developed to determine the distribution of stresses in such structures in order to select proper thickness in design of such tanks. A more accurate determination of thickness will impact safety, environmental and economic issues.

In this paper, general shell theory will be used to describe the shells of non-revolution. The governing equations of linear elasticity for shells of elliptical cross section will be developed. Then from the general equations, the system of equations for cylindrical shells of elliptical cross section under the action of internal pressure will be developed. These equations will be solved for normal forces, shear forces, and bending moments and a comparison will be made with finite-element results and existing analytical solutions.

A Second-Order Homogenization Method for Finite Elasticity

Castañeda, P.P.
University of Pennsylvania, USA

Homogenization theory deals with the characterization of the averaged or effective properties of composite materials. This theory is extremely useful in practice because it greatly simplifies the analysis of structural problems involving composite materials, especially, when the material microstructure and the relevant loading histories are complex. Many different homogenization techniques have been developed over the years for *linear* systems. In comparison, the development of homogenization methods for *nonlinear* media is still in its early stages, in spite of the fact that essentially all material systems exhibit one type of nonlinearity or another at sufficiently high field intensity. This paper is concerned with the development of a new homogenization procedure for *finite-elastic composite materials*. This class of materials presents a special challenge because their stored-energy density functions are *nonconvex*, as a consequence of the intricate coupling between the so-called "constitutive" and "geometric" nonlinearities. The procedure, which is based on the "second-order" procedure developed by the author for nonlinearly

viscous systems, seeks to estimate the effective stored-energy functions of finite-elastic composites in terms of suitably chosen "linear comparison composites" incorporating information about the constitutive response of the phases, as well as statistical information about their microstructures (such as volume fractions and two-point correlation functions). The development of the proposed effective constitutive models is important for the characterization of carbon-black filled elastomers in the car-tire and many other industries.

Session: E3-7 Room: Cascade 125 **Time:** W1:00p-3:00p
Chairs: *A. Wineman (U. Mich.) & J. F. Cárdenas (Texas Tech)*

Mechanical Response of Dry and Wet Sand to High Strain Rate Loading

Wilson, W.H.
Air Force Research Laboratory, USA
Tasker, D.G.
Los Alamos National Lab, USA
Dick, R.D.
University of Maryland, USA
Gustavson, P.K., Dieter, J.S. and Lee, R.J.
Indian Head Division, USA

High strain-rate mechanical properties of two types of sand, one a riverbed sand and one a beach sand, were studied using a modified split-Hopkinson pressure bar technique. Wet (near full saturation), partially saturated, and dry samples of each sand were confined in a thick-walled steel vessel and between the two steel pressure bars, and loaded at various strain rates. Some of the basic observations are that: 1) stress wave propagation was dominated by the void content; 2) dry sand crushed readily, yet void compression was incomplete; 3) water content reduced grain damage; 4) for low strain rates, large strains occurred at low stresses, but at high strain rates, small strains occurred at high stress; 5) sands containing approximately 10% gas needed a sustained stress of ~90 MPa to close the voids before significant stresses could be transmitted; 6) the applied pressure required for void compression increased with void content. In these samples, the bulk modulus before void compression was only of the order of 0.2 GPa, and then rose suddenly to approximately 6 GPa after compression and lock-up. Typical wave velocities observed were around 300 m/s before void compression, rising to around 1.6 km/s after compression. Based on the measurements, a simple model is presented for response of a 10% gas-content, semi-infinite sand space to shock loading, incident from a water interface.

The Practical Use of the Hole Method Using Moiré

Cárdenas-García, J.F. and Verhaegh, J.E.
Texas Tech University, USA

The use of a small circular hole in elasto-static photoelasticity to determine the stress tensor for any two-dimensional general loading situation is well known. A similar approach relying on the use of moiré to determine the strain tensor has not been implemented. The purpose of this paper is to report on the practicality of performing such a measurement. There are problems inherent to the use of moiré that need to be addressed and overcome, such as the fact that moiré relies on a pre-oriented grating for its measurement. This presents a problem because the orientation of the principal strain (stress) directions is not known before a hole is drilled on a specimen, therefore making it impossible to correctly pre-align the moiré gratings. Finding a solution to this problem is basic to seeking an acceptable approach to making the hole-method amenable to measurement by the moiré method. It would also be useful to develop an experimental approach that uses the majority of the fringe-order information that is available, away from the axes of symmetry.

Singular Problems in Elasticity: Linear vs. Nonlinear Theory

Aguiar, A.R.
Rice University, USA, and
Fosdick, R.L.
University of Minnesota, USA

This study concerns the local behavior of the solutions of the governing equations of elastostatics in the vicinity of corners. It contains an asymptotic investigation - within both the linear and nonlinear theories of plane strain - of the deformation field near a corner point that separates a free and a fixed part of the boundary. Numerical results confirm that the asymptotic solutions represent the local behaviors of equilibrium states very close to the corner. As we move away from the corner, the rates of deformation become small and the asymptotic solution in the nonlinear theory becomes - expectedly - not valid. Nevertheless, the numerical results obtained for both the linear and nonlinear theories show striking similarities and predict an unexpected behavior of the deformation field that is physically possible.

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the University of Minnesota Supercomputing Institute for their support of this research.

Experiments and Modeling of Nonlinear Coupling Effects in Elastomeric Bushings

Kadlowec, J., Wineman, A. and Hulbert, G.
University of Michigan, USA

Elastomeric bushings are structural components that isolate vibration, reduction noise transmission, accommodate oscillatory motions and accept misalignment of axes. A bushing is composed of an elastomeric hollow cylinder contained between an inner and an outer cylindrical sleeve. The bushings of interest in this study are used in automotive suspension systems. The steel sleeves connect components of the suspension system and transfer forces between the wheel and chassis while the elastomeric material reduces shock and vibration in this connection. During normal use, the bushing sleeves undergo displacements and rotations relative to one another about axes both along and perpendicular to the centerline of the sleeves. The relation between the forces and moments and their corresponding displacements and rotations is nonlinear viscoelastic due to the nature of the elastomeric material.

Experimental results are presented which explore the nonlinear interactions when the bushing undergoes a variety of transitional and rotational displacement modes. These modes are produced by displacement control tests. The specific tests are ramp to constant displacement at different rates and final displacements. The specific modes considered are radial, torsional and coupled radial and torsional. Results for the separate radial and torsional modes provide a database for uniaxial response. Combined radial-torsional results are compared to the result of superposing the two separate uniaxial responses. The combined response is found to be softer. The comparison brings out the strength of coupling and assesses its time variation. Data analysis is sued in determining the constraints in a proposed model for coupled, nonlinear viscoelastic bushing response. This consequent force-deformation relation is a useful approximation to account for coupling and will become an integral part of a multi-body dynamics model for an automobile suspension.

Evaluation of Viscoelastic Characteristics of Soft Stringy Foods

Nakajo, Y.
Ashikaga Institute of Technology, Japan

Taste of foods is greatly affected by their texture. To maintain the consistent quality of a soft food as a product, evaluation of its mechanical properties by sampling inspection is indispensable. Traditionally, the characteristics of the soft stringy foods such as noodles and pasta have been represented by their elastic moduli and maximum strengths in tensile tests or by rheological properties determined by texturometer or rheometer in compression tests. However, the former method does not give consistent results especially when the food has strong time-dependent characteristics and the latter one which requires expensive and exclusive test equipment offers unfamiliar physical data to a mechanical engineer.

The present paper proposes a simple and precise method to evaluate the material properties of soft stringy foods such as noodles. In the experiment Japanese wheat noodle, or "udon", is selected as specimen which is traditional but still quite popular food among all the generations in Japan like principal food, rice. In the study, specimen is hanged in catenary and the central deflection is measured every moment. By adopting this method, the tensile stress due to its tare weight distributes along entire length of the noodle and unevenness of the deformation is alleviated better than the case the noodle is hanged at one end. By assuming the phenomenon is quasi-static, the momentary compliance are calculated with the deflections. Then the compliance of the food is determined by fitting the curve to a well-known viscoelastic body. The results show that high-grade hand-made noodles require three-element viscoelastic standard solid model to fit the constitutive equations while relatively less-expensive machine-made noodles can be expressed by simple Maxwell model. Also, the author proposes a simplified calculation which reduces the complicated trigonometric and hyperbolic equations to a simple cubic equation by employing series expansion for use in a test at site. The accuracy is assured within 20% error and the results are consistent. Finally obtained viscoelastic parameters, elastic moduli and viscosity coefficients of the elements in the model, are related to sensuous valuations such as feel to the tongue or teeth. The proposed evaluation method provides simple inspection which gives consistent measured values and calculated results without no special equipment or calculation techniques, available both in the laboratories and at site.

Symposium E4
Mechanics and Materials Issues in Solid Polymers
Organizers
S. Ahzi
Clemson University, USA
&
M. Negahban
University of Nebraska, USA

Session: E4-1 Room: CUB 222 **Time:** M10:00a-12:00p
Chairs: *A. Wineman (U. Mich.) &*
A. Gusev (Inst. Of Polymers)

Toughness Jumps in Particle Modified Polymers

Argon, A.S.
Massachusetts Institute or Technology, USA

In many polymer systems ranging from semi-crystalline polymers such as polyamides (Nylon) and high density polyethylene with high levels of crystallinity to thermoplastic glassy polymers such as PMMA, PS and thermoset epoxies toughness jumps have been reported resulting from particle modification when the interparticle ligament dimensions become less than a certain dimension - depending on the specific system. The explanations for these phenomena differ but most often are based on the specific morphology of the matrix material and have little to do with the mechanical properties of the particles themselves. A number of well-defined examples in semi-crystalline polymers will be presented for which the information is complete. For other cases other possible mechanisms will be proposed and discussed.

Micromechanics of Particle-Toughened Semi-Crystalline Polymers

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The limited toughness of otherwise attractive semi-crystalline thermoplastics can be mitigated by incorporation of dispersed second-phase particles. Indeed, dramatic jumps in toughness have been observed upon reaching an optimal combination of particle size and particle volume friction. The observed jumps have been correlated with the achievement of a critical interparticle ligament distance. The correlation between toughness jumps and a material length scale indicates that purely continuum mechanics arguments cannot explain the dramatic jumps in toughness. There is experimental evidence that interface-nucleated crystallization from the melt results in preferred crystallographic textures in the matrix with chain axes primarily tangent to the interfaces. In turn, the comparative ease of chain and transverse slip on these planes provides high plastic anisotropy within a thin lamina of material surrounding the particle.

In this paper the role of the matrix morphology in controlling toughness is explored through micromechanical analysis. Finite element unit cell models which account for the anisotropic plasticity of the highly-textured material surrounding the particle are constructed and analyzed. The studies show that when the textured matrix morphology percolates the interparticle ligament, it alters the nature of the stress and plastic deformation fields around the particles, thus serving to toughen the semi-crystalline thermoplastic.

Microstructure, Mechanical Performance and Deformation Behaviour of Thermally Aged Polypropylene

Gensler, R., Plummer, C.J.G. and Kausch, H-H.
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Isotactic Polypropylene (PP) is very susceptible to thermo-oxidative degradation. It is therefore indispensable to stabilize any PP product in order to guarantee long-term performance [1]. Typical heat stabilizers for PP are phenolic antioxidants and hindered amine stabilizers (HAS). In order to determine the antioxidant efficiency, oven aging at elevated temperatures ($T > 110°C$) is the usual industrial practice. Under such conditions the degradation behaviour of HAS and phenolic stabilized samples differs significantly [2]. A phenolic stabilized sample shows a dramatic drop in mechanical performance after the end of an induction period, during which no apparent property changes can be detected. With HAS a gradual decrease in mechanical performance is observed from the outset. At low aging temperatures ($T < 100°C$), however, HAS may outperform phenolic antioxidants. Therefore, the results of accelerated aging at high temperatures may lead to erroneous estimations concerning the efficiency of HAS. In this work we have investigated the chemical and microstructural origins of the different degradation behaviour of phenolic and HAS antioxidants at high aging temperatures.

Different PP homopolymers and PP blends with varying molecular weights have been studied. For each material, two series of specimens were prepared, one containing a phenolic antioxidant (Irganox 1010, Ciba Specialty Chemicals, 0.05 wt.-%) and one containing a HAS (Chimassorb 944, Ciba Specialty Chemicals, 0.05 wt.-%). Samples for mechanical tests were aged at 120°C and 135°C in forced draft air ovens. The evolution of polymer degradation was monitored by the measurement of mechanical properties, DSC, FTIR, chemiluminescence, GPC and ESR. The microstructure and the deformation mechanisms were studied by TEM, SEM and optical microscopy. It was found that

the additive package has no influence on the mechanical properties, the crystallinity and the deformation behaviour of unaged samples. For aged samples, however, significant differences were observed. Within the first 10-15 days at 135°C the yield stress of HAS stabilized samples dropped to very low levels, and the modulus and the crystallinity increased. On the other hand, the properties of the phenolic stabilized samples did not change over up to 60 days. These results suggest that extensive chain scission occurred in the amorphous interlamellar regions in the HAS stabilized samples. This would facilitate reorganization of the PP chains at the lamellar surfaces, accounting for the increase in crystallinity and modulus. Further evidence for chain scission was obtained from GPC measurements and IR-spectroscopy. The evolution of the carbonyl absorbance at 1716 cm-1 correlated well with that of the mechanical properties.

The deformation mechanisms in undegraded and degraded samples have also been investigated. Phenolic stabilized samples showed no change in behaviour, the deformation mechanisms observed for aged samples being the same as for virgin samples. For the HAS stabilized samples, however, the deformation mechanisms changed dramatically within the first 15 days at 135°C, depending on the molecular weight of the starting materials. High molecular weight PP grades, which initially displayed highly ductile behaviour, underwent a transition from extensive shear deformation to sparse crazing in the most highly degraded samples. Low molecular weight PP grades deformed in the undegraded state by multiple crazing, but in the aged samples individual crazes became longer and the overall craze density decreased. These results are discussed in terms of the stabilizing mechanisms proposed in the literature and own ESR measurements.

[1] E.P. Moore, Polypropylene Handbook (Hanser, Munich, 1996).
[2] F. Gugumus, Polymer Degradation and Stability 44 (1994) 299.

Effect of Structure Property Relationships on the Electrical Conductivity, Mechanical Strength, and Optical Properties of Electroactive Polyaniline

Gregory, R.V.
Clemson University, USA

Fibers and films formed from organic inherently conductive polymers are finding wide spread applications in electronic and photonic devices. Polyaniline is of particular interest due to its facile processing under conditions normally associated with polymer processing and its high electrical conductivity. Recent work in our laboratory is beginning to shed light on the effect of the polymer morphology on the electrical, optical, and mechanical properties of the formed fiber and film. Measurements of the refractive indices in all three dimensions as well as the electrical conductivity transport mechanisms are shown to be highly dependent on the morphology of the fibers or film. The morphology is directly affected by processing variables such as orientation and solvent content. We will report on measurements of the optical properties, and electrical conductivity's obtainable under differing processing conditions. The effect of these processing conditions the developing polymer microstructure will also be discussed in detail.

Session: E4-2 Room: CUB 222 **Time:** M1:30p-3:30p
Chairs: *E. Arruda (U. Mich.) & R Seguela (U. Sci & Tech)*

Time-Dependent Viscosity and Physical Aging in Polymers and Polymer Composites

Zheng, S.F. and Weng, G.J.
Rutgers University, USA

The mechanical behavior of many polymers can be described by linear viscoelasticity, but when the visco-component - or the viscosity - of its viscoelastic property changes as a function of time, its behavior ceases to be linearly viscoelastic, and the well established correspondence principle could not be applied. Such a change is most easily conceived in physical aging during which the viscosity of the polymers continues to increase as a function of time. When such polymers serve as the matrix in a fiber-reinforced composite, the viscoelastic behavior of the composite system will also become nonlinear, and its effective viscoelastic property as a function of the fiber volume concentration will also become difficult to determine. In order to overcome such difficulties, a new theory is developed which allows one to convert the nonlinear viscoelastic problem into a linear one. The theory is based upon an "effective time" which is a function of the time-dependent viscosity. It differs from the "effective time" commonly introduced in the study of physical aging for the horizontal shift, but it is broad enough to cover such chrono-rheologically simple materials. To demonstrate its applicability to such simple materials, the theory of time-dependent viscosity is applied to describe the long-term creep of a Dow Derakane 470-36 thermosetting resin undergoing the aging process, and then coupled with a micromechanics theory to predict the long-term creep compliance of its composite reinforced with 30% of glass fibers.

The results are found to be in total agreement with the experimental data for both the pure resin and its composites. It should be kept in mind, however, that the applicability of the theory is likely to go beyond such simple materials.

Modeling of the Competition Between Shear Yielding and Brittle Failure by Crazing in Amorphous Polymers

Estevez, R. and Van der Giessen, E.
Delft University of Technology, The Netherlands

Although amorphous glassy polymers, like polystyrene (PS), styrene-acrylonotrile (SAN), polymethyl-methacrylate (PMMA) and polycarbonate (PC), usually fail in a rather brittle manner, there is an important class of these materials that may also undergo substantial plastic deformation by shear yielding. The subsequent shielding by the plastic zone can strongly influence the fracture resistance. Crazing and plastic shearing are often thought to be independent mechanisms. However, recent experiments (e.g. [1]) have shown that craze initiation in some polymers does not occur until the crack-tip plastic zone has developed to a critical extent. Therefore, a proper description of the plastic deformation zone near the crack tip is vitally important for the understanding of the fracture mechanisms in these polymers.

An earlier study [2] has focussed on the development of the plastic zone around a stationary crack tip. It has been demonstrated how the large strain plastic flow characteristics of amorphous polymers govern the shape and size of the plastic zone. Due to the intrinsic softening after yield, followed by the progressive orientational hardening at continued straining, the plastic zones develop quite different shapes than the familiar crack-tip plastic zones in metals. These computations also confirmed qualitatively the observations of [1].

This study proceeds from this by considering now a propagating crack. This is simulated using an embedded cohesive surface ahead of the crack. The constitutive behavior of the cohesive surface is designed to mimic the initiation, growth and final break-down of a craze. the model allows to study in detail the interaction of crack-tip plasticity with the mechanism of crack advance.

1. Yamamoto, T. and H. Furukawa (1995), Polymer 36, 2393=AD2396.
2. Lai, J. and E. Van der Giessen (1997), Mech. Mater. 25, 183-197.

Modeling Mechanical, Thermal, and Electric Properties of Composite Materials

Gusev, A.A.
ETH-Zentrum, Switzerland

Most industrial composite materials have random microstructure with inclusions of different size and shape forming an enormous variety of local microstructural configurations. We use Monte Carlo runs [1] to generate representative multi-inclusion models of actual composite materials. The composite microstructure is reproduced by periodic networks [1] of a few million and more non-overlapping tetrahedral covering space inside disordered unit cells without holes. Variational formulation is used to construct the total energy of these periodic models in the presence of external thermomechanical or electric fields. Assuming realistic phase properties, direct energy minimization [1] is employed for finding the overall thermomechanical and electric response as well as the underlying local fields in the composite constituents.

The computational efficiency and technological significance of the modeling approach taken are illustrated based on on-going collaborative efforts including matching the thermal expansion coefficients of polymer-based composites for automobile applications and steels, predicting the overall stiffness of polymers reinforced by high-aspect ratio carbon nanotubes, studying the initiation of local damage in carbon/epoxy and glass/epoxy composite for aviation and space technologies, modeling local strains in Al-Ni-Mo alloys, understanding dielectric properties of silicon-based foams, improving the efficiency of liquid-crystal displays, etc.

[1] A. Gusev, JMPS 45, 1449 (1997)

Modeling of The Elastic-Inelastic Response of Layered Sl5170 Resin Parts Produced by Stereolithography

Ahzi, S.
Clemson University, USA

Stereolithography (SL) is one of the processes used in rapid prototyping and manufacturing. In this process, selective photopolymerization (UV beam) is used to build parts, layer by layer, that can be either used as prototypes or functional parts. One of the current interests in the use of the SL process is the development of rapid polymer tools such as dies for injection molding. Both filled and non-filled SL5170 resins have been investigated for this purpose. In order to understand the thermo-mechanical response during loading and unloading of SL parts, we conducted a series of experimental tests to characterize the stress-strain response for large strains and for different temperatures. These tests were conducted on both non-filled and silica-filled SL5170 resin. We also implemented an elastic-viscoplastic model for the simulation of large deformation behavior of these materials. The experimental results as well as the model predictions will be presented and discussed.

Predicting Local Damage in Unidirectional Composites

Rozman, M. and Gusev, A.A.
ETH-Zentrum, Switzerland

Unidirectional boron/epoxy, glass/epoxy, or carbon/epoxy composites possess excellent strength and stiffness in the fiber direction and are indispensable today in many demanding applications

including aviation and since technologies. A critical constraint when using unidirectional composites is their low damage tolerance. Numerous attempts have been made to predict the appearance of local damage assuming a regular square or hexagonal packing array of fibers. The unit cells of these traditional models contain only one fiber which considerably simplifies the theoretical analysis. However, experimental investigations of the transverse cross sections of real unidirectional composites have not suggested anything other than a completely random packing array of fibers.

A Monte Carlo (MC) procedure was employed to generate statistically independent realizations of a periodic glass/epoxy and carbon/epoxy unidirectional composite with a disordered unit cell containing a random dispersion of 1024 perfectly-aligned fibers. Three dimensional variable-density meshes of up to a million triangular prisms were generated to approximate the composite's microstructure. Using a direct energy minimization approach, we numerically calculated the local stress concentrations accompanying transverse loadings. We have found that the maximum stress concentrations in the matrix take place inside thin bridges separating nearest fibers. For relatively large separations, i.e. larger than a percent or so of the fiber diameter, the stress concentrations were found to increase with decreasing bridge thickness. However a cross-over was seen at bridge thicknesses of ca. 0.1% and the local stress concentrations leveled off for thinner bridges. We propose to take the local stress concentrations inside the bridges as a single value parameter controlling the appearance of first local damage in composites and demonstrate its technological significance in different practical situations.

Session: E4-3 Room: CUB 222 **Time:** M4:00p-6:00p
Chairs: *M. Negahban (U. Nebraska) &*
M. E. Godard (U. De Rouen, France)

Time Dependent Deformation In Elastomeric Materials

Bergstrom, J. and Boyce, M.C.
Massachusetts Institute of Technology, USA

Elastomeric materials are known to exhibit time dependent deformation as evident in hysteresis and stress relation phenomenon. Here, experiments which explore various aspects of the time-dependence of the stress-strain behavior of elastomers are presented. A physically-based constitutive model which captures a wide range in observed behavior is presented and compared to experimental data. The influence of fillers such as carbon black is also discussed.

Structure-Property Relationship in Glassy Polymers Through the Tool-Moynihan-Narayanaswamy Relationship

Godard, M-E. and Saiter, J-M.
Université de Rouen, France

One of the most widely used equation to characterize enthalpy recovery in amorphous polymers is the Tool-Narayanaswamy-Moynihan empirical relationship:

$$\tau = \tau_0 \exp\left(\frac{x^{\Delta} h^*}{RT}\right)\exp\left(\frac{(1-x)^{\Delta}\ h^*}{RT_f}\right)$$

which defines a relaxation time τ by introducing, through the first term, the effect of temperature and the effect of structure with the second term. In this relationship, x is the non-linearity parameter, Δh^* is the apparent activation energy and T_f is the fictive temperature.

Even if a great amount of (x, Δh^*) data can be found in the literature, no direct correlations between these parameters and the engaged structure are available. Using some polymers in which structural changes are controlled and studying some recently published results, this problem may be overstayed. This is what we intend to do in this work where we study the influence, on the relaxation phenomena, of the length of the lateral chain in the polymethyl(α-n-alkyl) acrylates family and the influence of the connectivity in inorganic polymers.

Biaxial, Nonlinear Behavior of Solid Polymers

Lu, H-B. and Velvadapu, C.V.
Oklahoma State University, USA

The rate dependence of the yield-like behavior and the effects of volumetric and shear deformations in controlling the viscoelastic response rate are investigated under biaxial stress state. Plate Polymethal Methacrylate (PMMA) specimens are used in this study. Digital image correlation technique is used to measure the surface deformations when a combined isotropic and deviatoric loading is applied. This technique allows the measurement over a wide range of temperatures, including temperatures close to the glass transition. It is observed that a linear to nonlinear transition can be clearly identified from the isochronic stress-strain relation. The PMMA enters a nonlinear range at a strain level of 0.5% at any temperatures, indicating that the strain controls the transition from linear to nonlinear behavior. The biaxial yield-like behavior depends highly on the isotropic and deviatoric stress rates. Both isotropic and deviatoric deformations control the viscoelastic response rate. While shear alone increases the viscoelastic response rate, a positive volumetric deformation increases the deformation rate and a negative volumetric deformation decreases the viscoelastic response rate.

The role of volumetric deformation increases significantly over time and temperature. A modified nonlinearly viscoelastic constitutive model based on the effective fractional free volume is proposed to explain the behavior observed in the experimental investigation.

Monte Carlo Modelling of Polymer Deformation

Chui, C. and Boyce, M.C.
Massachusetts Institute of Technology, USA

In recent years, there has been much success in the development of physically based continuum level constitutive models of the elastic-viscoplastic behavior of amorphous polymers. These models are based on hypotheses regarding the underlying deformation mechanisms of the polymer. In this paper, we present a monte carlo model of the amorphous polymer macromolecular network structure and its deformation. The stress-strain behavior is computed under a variety of deformation conditions. The inter- and intra-molecular contributions to the stress-stain behavior are identified and discussed. Particular regard is given to the relevance of continuum level modeling assumptions and their connection to observations from this molecular level model.

AFM Observation of Microscopic Behavior of Glassy Polymer and Constitutive Modellings

Tomita, Y., Adachi, T. and Tanaka, S.
Kobe University, Japan

A polymer under drawing is significantly hardened in the drawing direction due to the orientation of the molecular chain and thereby exhibits the neck propagation. To duplicate the characteristic feature of polymeric material, the molecular chain network models have been widely developed under the hypothesis that the molecular chain network structure deforms together with the bulk material. The validity of these models has been examined through a comparison of the computationally predicted macroscopic deformation behavior with that obtained by the experiments. However, the detailed discussion concerning the adequacy of the hypothesis in the micro level has not yet been clarified.

In this investigation, an atomic force microscope (AFM) observation on the surface of polycarbonate (PC) specimen under tension and simple shear have been performed to investigate the micro- to macroscopic deformation behavior of the surface of the PC. It has been clarified that a wavy microfibril structure aligned along the principal stretch direction is formed on the surface and the structure is subdivided to form a thin microfibril structure as the deformation proceeded. The rotation of the aligned microfibril structure, the aggregate of molecular chains, formed on the surface of deformed specimen slightly lags behind that of the principal direction of plastic stretch of bulk material. This suggests the validity of the hypothesis in approximate sense for the stretch predominant deformation. On the other hand, the necessity of more elaborate constitutive model accounting for the above indicated experimental evidence is implied. The remaining part of present paper is concerned with the generalization of the constitutive equation based on the molecular chain network theory to that account for thus clarified experimental evidence. Through the finite element simulation with newly developed constitutive equation, the effect of the relaxation of the hypothesis set to the deformation of the molecular chain structure and the bulk material on neck and shear band propagation behaviors is discussed.

Session: E4-4 Room: CUB 222 **Time:** T9:30a-11:30a
Chairs: *G. Weng (Rutgers) & R. Gregory (Clemson)*

A Model For Stress Evolution During Thermoset Cure

Mei, Y., Wineman, A. and Yee, A.F.
University of Michigan, USA

A constitutive equation is presented which accounts for stresses developed during the curing of epoxy. The continuous creation of new cross links after the chemical gelation point forms new networks which can transmit stress. Each new network has a different reference configuration due to volume changes of previously formed networks. The mechanical response of each new network is assumed to be linear viscoelastic if the cure temperature is around Tg. The rate of formation of the new networks depends on the rate of curing. The total stress at any instant is the superposition of the stresses from each network formed from gelation until that instant.

Using a curing rate based on experimental evidence, the model is used to determine chemical shrinkage under isothermal cure. Simulations are carried out for various assumed material parameters. The results are in qualitative agreement with experimental data.

A Viscoelastic Cohesive Zone Model for Application to Crack Growth in Polymers

Allen, D.H.
Texas A&M University, USA

One method of accounting for such enigmatic problems as r-toughening and subcritical crack growth that has come under recently increasing scrutiny is the approach of implementing a cohesive zone at the crack tip, following the early works of Dugdale and Barenblatt. In this method, a zone of non-zero tractions is placed at the crack tip, often thereby removing the stress singularity. A particularly inviting aspect of this approach is that, depending on the

constitutive model used for the traction-displacement relationship along the crack faces, history dependence can be incorporated into the critical energy release rate as a predictive capability in fatigue models. Unfortunately, the choice of a constitutive model for the cohesive zone is the weakest part of this approach to the fracture mechanics problem. Due to the small scale of the actual cohesive zone in most materials, it is experimentally quite difficult to determine the precise nature of the constitutive behavior in the cohesive zone. Thus, it has become commonplace to postulate a phenomenological form for the cohesive zone constitutive model that contains one or more free parameters, and while this approach has been shown to qualitatively predict some phenomena that have not been explained by analyses involving singular stress fields and/or constant critical energy release rates, the inability to construct physically based cohesive zone models has impeded this approach.

A micromechanical framework for developing continuum descriptions of viscoelastic cohesive zones at crack tips is discussed herein. This is accomplished by starting with a three dimensional continuum mechanics description of the cohesive zone that contains geometric descriptors of the structure of the cohesive zone. This micromechanics problem is then solved and a homogenization principle is utilized to construct a mechanical constitutive model for the viscoelastic cohesive zone wherein the failure of the cohesive zone is reflected through the use of an internal variable, thus producing a constitutive model for the traction-displacement relation that is simultaneously of single integral and internal variable type. The model is then shown to be consistent with the concept of a path independent integral for the available energy for crack growth, but with a critical energy release rate that is not a material constant. The paper concludes with an example analysis using the model.

Computer Simulation of Bimodal Elastomer Networks

von Lockette, P.R., and Arruda, E.M.,
University of Michigan, USA

Bimodal elastomeric materials are gaining increasing notoriety for their improvements in toughness and ultimate strength properties over their unimodal counterparts. Research into the nature of these increases has focused on aspects of the network structure and shared load bearing among the constituents. This work offers preliminary results of a new bimodal elastomer network simulation program which employs a realistic crosslinking scheme, following the elegant work of B.E. Eichenger on unimodal systems. Boundary constraints and edge effects, which can produce systemic errors in results, are eliminated through the use of periodic boundary conditions allowing for smaller simulation cells and reduced computational costs. Diagnostics performed on the resultant bimodal network structures assess sol fraction, gel fraction, and defects versus material composition. Results of unimodal simulations using the program are compared to previous simulated results on unimodal networks found in the literature. The authors also search for structural patterns in the sub-networks formed by the viewing each of the material's components separately in the gel.

Microvoid Growth in a Sphere of Elastomeric Material Exhibiting Strain-Dependent Damage

Huntley, H.E. and Wineman, A.
The University of Michigan, USA

A sphere of initially isotropic, homogeneous, nonlinearly elastic material is subjected to a uniform radial tensile traction. A traction-free spherical cavity or microvoid is assumed to exist at the center of the sphere. This problem has been studied previously assuming elastic material and, in other work, assuming elastic-perfectly plastic material. In the present work, a constitutive equation is used which postulates a continuous process of strain-dependent microstructural change. Two cases are considered: (1) Original microstructures break down and release their stress, and are replaced by new microstructures with different reference configurations. This results in stress softening and permanent set. (2) Original microstructures are not replaced as they rupture. This implies increasing loss of stiffness.

The stress distribution during loading and residual stresses upon release of external traction are examined. Load-expansion relations are evaluated for both cases (1) and (2). Permanent deformation after unloading is considered.

Scratching Behavior of Elastomeric PDMS Coatings

Zhang, S.L.
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Tsou, A.H.
Eastman Kodak Company, USA and
Li, J.C.M.
University of Rochester, USA

Scratch testing was performed on the elastomeric poly(dimethylsiloxane) (PDMS) coatings on steel substrates using spherical sapphire (76 μm radius) and conical diamond (136° apical angle) indenters. Both to horizontal force and normal load during scratch testing were measured. The morphology of scratches was examined using scanning electron and optical microscopes.

With increasing normal load during scratching, the friction coefficient (horizontal force/normal load) using a spherical indenter decreases while it appears almost constant using a conical indenter. The results can be

explained by recognizing that during scratching the contact area is determined by elastic deformation that the frictional force may be proportional to the contact area. With increasing scratching speed, the friction coefficient increases but the rate of increase of the coefficient becomes less, suggesting that the scratching of the FDMS coating is a rate process and the viscoelastic property of the coating influences its frictional behavior. Below a critical normal load which increases with the coating thickness the PDMS coating recovers elastically after being scratched. Above the critical normal load, the coating is damaged due to a combination of delamination at the coating/substrate interface and through-thickness cracking. The delamination of the coating from the substrate is evidenced by the exposed steel substrate under SEM and the fact that bulk PDMS material can only be damaged at a much higher normal load. The result that the critical normal load increases with coating thickness is also consistent with the delamination mechanism. When the coating is damaged there is an increase in the friction coefficient and a stick-slip motion occurs. It was also found that the increase in scratching speed enlarges the critical normal load. The critical normal load appears related to the interfacial strength of the coating.

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Session: E4-5 Room: CUB 222 **Time:** T1:00p-3:00p
Chairs: *M. Boyce (MIT) & S. Ahzi (Clemson)*

The Role of Long-Term Solutions in Modeling Inelastic Behavior of Solid Polymers

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Rensselaer Polytechnic Institute, USA

Room temperature experiments on commercially available Nylon 66, poly(etherether ketone), PEEK, and poly(etherimide), PEI, were performed with a servo-controlled testing machine. The extensometer was mounted on the gage length and enabled accurate strain measurement and control. If the material was ductile enough strains of 30% were reached. Several common features were found. Included are, nonlinear loading rate sensitivity, creep (stress rate is zero) and relaxation (rate of deformation is zero). The relaxation rate increases nonlinearly with an increase of the rate of deformation prior to the commencement of the relaxation test. When the relaxation tests are started in the region of fully established inelastic flow the relaxation curves, i. e. the stress drop vs. time curves, can be congruent. Then they are independent of the stress and strain at the start of the relaxation test. This feature is unusual and does not appear to have been noticed.

A modified state variable theory derived from the viscoplasticity theory based on overstress (VBO) was chosen for modeling. The theory consists of a set of coupled, nonlinear, stiff, first order differential equations. In one version the inelastic rate of deformation is only a function of the overstress, the difference between the stress and the equilibrium stress which is a state variable of VBO. For a test with constant rate of deformation this theory admits a long-time asymptotic solution for which the overstress is constant. This solution is thought to apply to the region of fully established inelastic flow. In this form of VBO the stress rate in a relaxation test depends only on the overstress. It follows that the predicted relaxation curve in the region where the long-term solution is applicable is independent of the stress and strain at which the test starts.

It appears that the existence of a long-term solution can correspond to a fully established inelastic flow in an experiment. It enables the modeling of observed, unusual inelastic deformation behaviors. It is also useful in finding the material constants from experimental results.

Inelastic Behavior of Polymers Under High Pressure

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Constitutive characterization of materials under large inelastic deformations is typically complicated by the onset of non-homogeneous deformation - shear banding, necking and fracture in tension, shear banding, barreling and/or buckling under compression. Friction on the loading plattens also plays a significant role when large compressive deformations are imposed. We present an experimental configuration where the complete state of stress and strain in the specimen are determined through direct experimental measurement, without a *priori* constitutive assumptions regarding the constitutive behavior of the specimen. Moreover, the control of the deformations is such that the deformations are always stable. Design considerations in implementing such an experimental configuration and applications to the investigation of pressure dependent yielding behavior in materials are also described.

The specimen considered is a cylindrical rod of diameter 2a and length *L*. It is inserted into the cavity of a hollow cylinder of internal diameter 2a and outer diameter *2b*. It is assumed that the deformation in the cylindrical specimen is homogeneous. The material of the confining cylinder is chosen such that it provides the necessary elastic restraint to the specimen and deforms elastically during the entire deformation of the specimen; the cylinder must also retain sufficient

compliance so as to enable measurement of its deformation during the test. The cylindrical specimen is strained by inserting a plunger into the cavity and displacing it by a loading frame to generate a compressive axial strain ε_{zz} of magnitude ε_0. The corresponding axial stress, σ_{zz}, can be measured easily using the load cell in any standard tensile testing machine. The confining cylinder provides an elastic restraint against the radial expansion of the specimen, thereby generating a radial pressure on the inner surface of the confining cylinder. The main idea of the constraint is to provide stability to the deformation; in the absence of this elastic restraint, barreling deformations can and do develop. Note that the radial pressure may also be provided by performing the test in a liquid under high pressure; there are a number of experiments in the literature that deal with the response of materials under hydrostatic pressure, beginning with the work of Bridginan. A large number of investigators have examined the pressure dependence of the mechanical properties of polymers. However, hydrostatic pressure from a liquid medium does not stabilize the deformation; in other words, the hydrostatic pressure does not prevent the barreling instability in a uniaxial compression specimen. On the other hand, the confined compression configuration that is suggested here ensures that the cylindrical deformation is stable. Results of this investigation are interpreted in terms of the multi-axial inelastic constitutive behavior of polycarbonate, with special reference to localization of deformation.

Plastic Behavior of Polyethylene and Related Copolymers in Terms of Uniform and Localized Crystal Slip Processes

Séguéla, R., Gaucher-Miri, V. and Elkoun, S.
Universite des Sciences et Technologies de Lille, France

Polyethylenes and related copolymers display double yield points depending on crystallinity and deformation conditions. The phenomenon is interpreted in terms of two thermally activated mechanisms of plastic deformation having quite different activation parameters, so that their flow stress is more or less sensitive to temperature and strain rate. The strain-hardening beyond each yield point depends on the nature of the mechanism activated. In addition, as crystallinity decreases, the lower temperature limit for the occurrence of a double yield point decreases and the higher strain rate limit increases. This effect parallels the temperature and frequency sensitivities of the crystalline mechanical relaxation. It stresses the correlation between viscoelastic and plastic processes at a molecular scale.

The two mechanisms competing in the plastic flow are ascribed to a homogeneous (otherwise uniform) crystal slip and a heterogeneous (otherwise localized) crystal slip, while the amorphous phase only plays a part of stress transfer agent. The former process is strongly temperature and strain rate sensitive and is characterized by a strong strain-hardening. It is associated with the ability of the material to develop macroscopically homogeneous plastic deformation. The model of homogeneous nucleation of screw dislocations from the lateral surfaces of the crystalline lamellae appeared as a good candidate to stand for the homogeneous crystal slip.

The second process of heterogeneous slip is the precursor to the plastic instability when the actual strain rate affordable from nucleation and propagation of dislocations is not high enough to match the macroscopic applied strain rate. The defective regions in the mosaic block structure of the crystalline lamellae can be suspected to concentrate the slip owing to the reduced molecular interactions in the misfit interface. The dissociation of the screw dislocations into partials propagating at lower shear stress than perfect dislocations may also be active. Indeed, such partial dislocations leave behind them a stacking fault that may play the same role as the above mentioned defective regions. Comparison of the two models predicts a stronger temperature-sensitivity for homogeneous slip together with a significant crystal thickness dependence.

The parallel between plasticity and viscoelasticity allowed us to proposed a molecular mechanism of dislocation nucleation and propagation based on a relaxation molecular model. Dissociation of screw dislocations is also discussed and an explanation is provided for the occurrence of martensitic phase change.

Thermomechanical Modeling of Crystallization in Polyethylene for Use in Simulation of Rotational Molding

Negahban, M.
University of Nebraska, USA

Rotational molding, a process commonly used for making large shell like structures, involves the melting of polymer powder (normally polyethylene) onto the hot internal surface of a mold while the mold is rotating slowly in an oven, and then cooling the mold and polymer to complete the process and remove the part Even thought the polymer undergoes very small deformations in this process, the cycle time of producing parts with this process is strongly influenced by the processes of fusion and crystallization in the polymer and their associated mechanical effects. For example, premature separation of the polymer from the mold will result in an insulating layer that will retard the cooling process and substantially increase the cycle time

A preliminary model for capturing the effects of crystallization and fusion in polyethylene will be introduced and its characteristics studied. This model will be based on a structure similar to that proposed

earlier for solid-solid phase transitions [1,2], but modified to capture solid-fluid transitions.

1. M Negahban, "Thermodynamic Modeling of the Thermomechanical Effects of Polymer Crystallization: A General Theoretical Structure," International Journal of Engineering Science, vol.35, 1997, pages 277-298
2. M. Negahban, "Thermomechanical Effects Associated with Crystallization of Rubber Under Stretch and During Slow Extension," Journal of Engineering Materials and Technology, vol.119, 1997, pages 298-304

Application of Drag Reducing Polymer in Energy and Water Saving in Sprinkler Irrigation Systems

Khalil, M.F., Elmiligui, A. and Naoum, F.
Alexandria University, Egypt

Sprinkler irrigation systems are now successfully applied in irrigation Schemes. Uniformity of water distribution, good application efficiency, limited erosion, relatively low labor requirement, and the practicability of use on various soils are attributes that make sprinkler irrigation as an efficient irrigation system. Furthermore, in many areas the water and energy required for irrigation are scarce, hence irrigation systems must apply water adequately and efficiently with less energy consumption. It has been shown that the evaporation loss may accounts as 20% to surrounding environment.

In this work trials are presented to reduce the pumping energy consumed to overcome pipe friction and also to reduce the evaporation loss to the environment during the spraying process. Experiments were carried out to study the effect of adding a drag reducing polymer, Sodium Carboxymethyl Cellulose-CMC-7H, on the evaporation loss of water droplets similar to that in sprinkler irrigation systems. The experiments were carried out in the subsonic wind tunnel at Alexandria University on a water droplet suspended in a stream of air where the dry bulb temperature T = 18.0^0 - 20.0^0 C, free stream velocity V = 1 - 8 m/sec, drop diameter d = 0.7 - 3.2 mm, and CMC-7H concentration = 20 - 1000 PPM. It was found that the evaporation loss increased with increasing dry bulb temperature, free stream velocity and decreased drop size. The addition of small quantities of polymer, 20 & 50 PPM, to the water droplets resulted in a considerable reduction in the evaporation loss. The percentage decrease in the evaporation loss becomes less effective with increasing CMC-7H concentration, more than 50 PPM. This study indicates that the drag reducing polymers can be applied in sprinkler irrigation system to save pumping energy in piping network as well as a water saver by reducing evaporation loss during the spraying process.

Symposium E5
Viscoelasticity in Composites
Organizer
D. Allen
Texas A&M University, USA

Session: E5-1 Room: CUB 208 **Time:** T3:30p-5:30p
Chairs: *D. Allen (Texas A&M U)*

Viscoelasticity in Composites

Schapery, R.A
University of Texas at Austin, USA

Composites with polymeric constituents exhibit appreciable time-dependent behavior over a wide range of service conditions. Viscoelasticity is a major source of this time-dependence, and must be taken into account to predict structural life or durability. In this talk I will discuss recent experimental and theoretical developments related to processing, hygrothermal environment, physical aging and high stresses. Understanding and modeling of time-dependent microcracking is an important part of durability analysis, but experimentally-validated models are still practically non-existent. The last part of my talk will be concerned with this problem area.

A Continuum Theory of Cohesive Zone Models

Costanzo, F.
Pennsylvania State University, USA

Various experimental investigations in dynamic crack propagation show that in several amorphous polymers

1. cracks, at the onset of fracture, seem to jump from the rest configuration to a steady state motion without a transitory smooth acceleration phase;
2. once crack start to propagate, its velocity remains essentially constant, ranging between 40% and 60% of the Rayleigh wave speed;
3. as the crack approaches its maximum value, its velocity is believed to oscillate rapidly and post-mortem surfaces display a periodic microstructure.

These phenomena have yet to be given a convincing theoretical explanation. However, the available experimental evidence seems to indicate that the characterization of the complex microstructure surrounding the crack front is the key to understanding the observed behavior. This is the rationale behind the recent increased interest in cohesive zone models and their application to the study of dynamically propagating crack linear-elastic media. The constitutive behavior of these models is often chosen to be rate dependent and non-linear. In spite of their new popularity, rigorous continuum mechanics studies of cohesive zone models are still in their early stages of development. Another aspect that needs to be developed is a micromechanics of those physical microstructures, such as polymer crazing, that are often modeled via cohesive zones.

In this paper a general three-dimensional continuum constitutive theory of cohesive zone models is presented. The main thrust of this work is the establishment of a systematic procedure for deriving cohesive interphase constitutive equations where crack deformation is accounted for not only via the opening displacement but also via crack surface strain tensors. The material frame indifference axiom is used to show that in traditional cohesive zone models where the opening displacement is the only crack deformation descriptor cohesive forces must be pointwise parallel to the opening displacement itself. This result indicates that the use of additional crack surface strain measures is required for the description of realistic crack tip microstructures with possible anisotropic behavior.

Micromechanical Analysis of a Granular Viscoelastic Composite

Allen, D.H.
Texas A&M University, USA

Herein a micromechanical analysis is performed on a granular composite composed of an elastic fiber and a viscoelastic matrix material. Since the grains are of variable size and shape, two approaches are utilized and compared. First, a generalized self-consistent scheme is used wherein the grains are idealized as spheres. A solution is obtained by utilizing the viscoelastic correspondence principle in conjunction with the elastic solution. Second, a Voroni cell generator is used to construct a random finite element mesh, and a solution is obtained with the finite element technique. These results are compared, and it is found that significant differences are obtained between the two solutions.

Session: E5-2 Room: CUB B1-5 **Time:** W9:30a-11:30a
Chair: *D. Allen (Texas A&M U)*

Nonlinear Anisotropic Piezo-Electro-Thermo-Viscoelasticity with Applications to Composites Plates

Hilton, H.H.
University of Illinois at Urbana-Champaign, USA
Vinson, J.R.
University of Delaware, USA, and
Yi, S.
Nanyang Technological University, Singapore

Piezoelectric effects are of importance in the control and sensing of structural element deflections. Elastic piezoelectric theory has been extensively developed,[1] but only a limited number of analytical and experimental publications on linear piezo-viscoelastic materials may be found in the literature. Aging effects

in composites are beginning to receive serious analytical and experimental attention, but no published data seems available on aging of piezo-viscoelastic materials.

In the previous paper, the authors developed the general nonlinear 3-D large deformation theory of anisotropic, nonhomogeneous piezo-electro-thermo-viscoelasticity. In addition to piezoelectric contributions, the anisotropic nonlinear viscoelastic constitutive relations include thermal expansion, curing and aging effects. Analytical and numerical solutions strategies are also discussed.

The generalized large elastic deformation constitutive relations with thermal expansions were first developed and then extended to corresponding nonlinear viscoelastic conditions to yield

$$\tau_j^i(\theta,t) = \int_{-\infty}^{t} \frac{\partial \phi_{jl}^{ik}(\theta,t,t')}{\partial t'} \gamma_k^l(\theta,t')dt'$$
$$- \int_{-\infty}^{T} \frac{\partial \phi_{jl}^{iE}(\theta,t,t')}{\partial t'} \mathbf{E}^l(\theta,t')dt'$$
$$- \int_{-\infty}^{t} \frac{\partial \phi_{jl}^{ik\mathbf{T}}(\theta,t,t')}{\partial t'} A_k^l T(\theta,t')dt'$$
$$- \int_{T*}^{T} \phi_j^{i\text{th}}(0,t,t')dt' - \int_{\alpha*}^{\alpha} \phi_j^{i\text{ch}}(\theta,t,t')dt' \qquad (1)$$

and

$$D^i(\theta,t') = \int_{-\infty}^{t} \frac{\partial \phi_l^{ikE}(\theta,t,t')}{\partial t'} \gamma_k^l(,t')dt'$$
$$+ \int_{-\infty}^{t} \frac{\partial \phi_l^{iE}(\theta,t,t')}{\partial t'} E^l(\theta,t')dt' \qquad (2)$$

Where τ_j^i are the Cauchy stress tensors, γ_k^l the Green-Zerna large strain tensors, ϕ_{jil}^{ik} the structural material, ϕ_{jk}^{iE} the electrical stiffness and ϕ_k^{iE} the dielectric permittivity relaxation functions with E^k the electrical field intensity vectors, $A_k^l T$ the thermal expansions and D^i the electric displacement vectors in spatial intrinsic curvilinear coordinates $\theta = (\theta^1,\theta^2,\theta^3)$ and in time t. The expressions $\phi_{jl}^{ik\text{th}}$ are thermal anisotropic relaxation functions, $\phi_{jl}^{ik\text{ch}}$ are chemical shrinkage anisotropic relaxation functions and $T*(\theta,t*)$ and $\alpha*(\theta,t*)$ respectively are stress-free reference temperatures and the corresponding degrees of cure. The last two integrals in Eqns 1 are only present during manufacturing processes and need to be included during service conditions. All these relaxation functions depend on environmental conditions and in the nonlinear case on strain rates and electrical intensity, such that any $\phi = \phi[\theta,t,t',M(\theta,t'),T(\theta,t'),$ $\alpha(\theta,t'),\dot{I}(\theta,t'),I_l^{\mathrm{E}}(\theta,t')]$, with M the moisture content, $\dot{I} = \{\dot{I}_i(\theta,t)\}$ the three fundamental strain rate invariants, $I_1^{\mathrm{E}} = tr\{E^k\}$ and $\alpha(M,T)$ the degree of cure. During cure $0 \le \alpha \le 1$, but while in service α equals unity and makes no contribution to any portion of the above relations.

Any and all of the above nonlinear anisotropic relaxation functions can be generally defined as

$$\phi_{jl}^{ik}(\theta,t,t',t_e,M,T,\alpha,\dot{I},\dot{I}^{\mathrm{E}}) = \qquad (3)$$
$$\sum_{m=0}^{M\frac{ik}{jl}} \sum_{p=0}^{P\frac{ik}{jl}} \sum_{q=0}^{Q\frac{ik}{jl}} \sum_{r=0}^{R\frac{ik}{jl}} B_{jlmpqr}^{ik}(\theta,t,t',t_e,M,T,\alpha)(\dot{I}_2 - 3)^{\mathrm{m}}$$
$$(\dot{I}_2 - 3)^{\mathrm{P}}(\dot{I}_3 - 3)^{\mathrm{q}}(\dot{I}^E - 3)^{\mathrm{r}}$$

where underscores indicate no summations over the affected indices, and where the parameters $\mathbf{M}_{jl}^{ik}, \mathbf{P}_{jl}^{ik}, \mathbf{Q}_{jl}^{ik}$ *and* $\mathbf{R}_{jl}^{ik}$ and the functions B_{jlmpqr}^{ik} are material dependent and represent distinct functional sets for each of the directional $\phi_{jl}^{ik}, \phi_{jl}^{iE}, \phi_l^{ikE}, \phi_j^{iE}, \phi_{jl}^{ikT}, \phi_j^{ith}$, and ϕ_j^{ich}, which must be experimentally generated for each material and environmental condition. Since the curing time scale is relatively short (about 300 min), the degree of cure α and the manufacturing process relaxation functions ϕ_j^{ith} and ϕ_j^{ich} are unaffected by t_e, the aged time. For linear materials, none of the parameters are dependent on any of the invariants of strains and/or of the electric field intensity and displacement. Additionally, for small deformations the stresses τ_j^i and strains γ_j^i reduce to their Cartesian engineering counterparts σ_{ij} and ε_{ij} and $x_i = \theta^i$.

For linear materials and small deformations, a piezoelastic/piezo-viscoelastic analogy was established in terms of integral Fourier and Laplace transforms. These analytical results are now applied to composite layered viscoelastic plates with piezoelectric viscoelastic strips on the top and bottom surfaces. In order to demonstrate the effectiveness of these piezo-viscoelastic constitutive relations, numerical examples of plate deformations and voltages under steady-state and sinusoidal loads are presented. Representative piezoelectric voltages generated by these configurations indicate that the distinct viscoelastic contributions of the plate and piezoelectric strips induce time decays in piezoelectric voltage responses. These results are also of importance in inverse problems, where voltages may be input to generate controlled displacements as prescribed by Eqs. (2). Conversely, such voltages can be used to control viscoelastic deformations and failure envelopes of composite structural elements.

[1]See Hilton, H.H., Vinson, J.R. and Yi, S., "Anisotropic piezo-electro-thermo-viscoelasticity theory with applications to composites," *Proceedings of the Eleventh International Conference on Composite Materials (ICCM-11). Gold Coast, Australia. July 14-18, 1997* for an extended bibliography and discussion

Constitutive Modeling of Polymeric Composites Undergoing Curing

Wang, K., Lagoudas, D.C., Whitcomb, J.D. and Allen, D.H.,
Texas A&M University, USA

An anisotropic viscoelastic model for polymeric fibrous composites undergoing curing will be discussed. The thermorheological constitutive model uses a reduced time influenced by the degree of curing. Recursive relationships were developed to permit an incremental form suitable for finite element analysis. A micromechanical analysis was performed using an hexagonal periodic array of fibers to obtain the monolayer effective response. After the effective response for monolayers was derived, for given matrix and fiber properties, a lamination procedure was developed to obtain the effective viscoelastic response of thick composite laminates.

Numerical Prediction of the Response of a Viscoelastic Laminate to Thermal-Mechanical Loading

Groves, S.E.
Lawrence Livermore National Lab, USA,
Zocher, M.A.
Los Alamos National Lab, USA and
DeTeresa, S.J.
Lawrence Livermore National Lab, USA

In order to conduct the analysis, the authors have developed a three dimensional orthotropic linear thermoviscoelastic finite element program (ORTHO3D) suitable for the analysis of composite structures subjected to a wide variety of loading histories. This program was developed in part to help predict the potential life times of high temperature composites for the proposed High Speed Civil Transport. An extensive data base of mechanical responses was generated under a DOE CRADA with Boeing Commercial Airplane Group, including thermo-mechanical fatigue and long-term creep of K3B/1M7 composite laminates. This work is presented as much for the purpose of demonstrating some of the capabilities of this new finite element program as it is for presenting the results of the mechanical studies.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Micromechanics Modeling for Viscoelastic Polymeric Composites – Interphase Effects

Brinson, L.C. and Fisher, F.
Northwestern University, USA

This study uses two different micromechanics approaches to investigate the overall mechanical property prediction for composites with finite interphase regions separating the inclusion and matrix materials. Interphase regions are often neglected in the analysis of elastic composites due to their relatively small volume fractions. However, polymer composites may possess much larger interphase regions which could influence the overall mechanical behavior of the material. Hence analytical models which accurately capture this behavior could prove quite useful from a design standpoint.

The first of the micromechanics models analyzed here was the popular Mori-Tanaka method, extended to the viscoelastic domain. This model assumes ellipsoidal phases embedded in a binding matrix, which allows the stress fields in the phases to be determined. For the current work this model was simplified by assuming that both the inclusion and interphase regions are ellipsoidal, thus losing the interpretation of the interphase as an annular region surrounding the inclusion. One of the goals of this work is to determine the impact of this assumption on the mechanical behavior predicted by this model.

The second micromechanical approach used in this analysis is based on the work of Benveniste. For this method the "auxiliary" problem of a coated inclusion embedded in an infinite medium of matrix material is solved initially. This is accomplished by finding suitable forms of the phase displacements in terms of a set of unknown constants. Using stress-strain and strain-displacement relationships along with enforcement of the boundary conditions and compatibility, these unknowns may be determined. The stress fields are then averaged to estimate the overall effective behavior of the composite. Thus using the Dynamic Correspondence Principle allows Benveniste's classic solution to be extended for viscoelastic materials.

Finally, a viscoelastic finite element analysis was undertaken to provide a baseline for comparison of the results of these models. This work will determine if either of these analytical models sufficiently captures the complex composite behavior predicted by a detailed FEM analysis. Such a model will be useful in providing a quick estimate of the overall behavior of a three-phase composite material of known material properties, and in solving the inverse problem to determine the unknown properties of an interphase region given overall composite properties.

Symposium F1
Inelastic Deformation and Failure. Symposium to Celebrate Professor E. Hart's 80th Birthday
Organizers
H. Garmestani
Florida State University, USA
&
F.G. Kollmann,
Tech. Hochschule Darmstadt, Germany

Session: F1-1 Room: CUB 224 **Time:** M10:00a-12:00p
Chairs: *F. G. Kollman (Tech. Hochschule Darmstadt) & John Cahn*

Stress Relaxation and Strain Aging in Intermetallic TiAl

Mecking, H., Willems, S. and Bartels, A.
Technische Universität Hamburg-Harburg, Germany

Like many intermetallic aluminides also Ti-48Al-2Cr exhibits anomalies of the rate sensitivity and temperature dependence of the yield stress at medium temperature. Unlike ordered Ni-Al and Fe-Al alloys, however, in TiAl dislocation pinning by a strain aging mechanism seems to play a more dominant role than intrinsic effects of the order on dislocation mobility. There are various different macroscopic effects which point at strain aging processes such as

- yield points after stress relaxation tests which continuously increase with relaxation time,
- a total standstill of relaxation following a rather rapid initial relaxation rate,
- a decrease of the yield stress with increasing deformation rate after an instantaneous ,
- positive stress jump immediately after a sudden increase of deformation rate,
- serrated flow in distinctive regimes of the flow curves in certain ranges of temperature and strain rate,
- suppression of dynamic recovery in the same range.

A quantitative study of these effects will be presented. It leads to the conclusion that material behavior is controlled by a diffusive process, most probably, interstitial diffusion.

Application of Modern Time Integrators to Hart's Model

Kirchner, E. and Kollmann, F.G.
Darmstadt University of Technology, Germany

Two time integration methods published recently by Freed & Iskovitz [1] and Kirchner & Simeon [2] are applied to the viscoplastic model of Hart [3] which is known to be hard to integrate even in the uniaxial case, Cordts & Kollmann [4]. A comparison of the computational performance is given for both methods.

To achieve consistency between the integrators and to fulfil the requirements proposed by Kirchner & Simeon [2] a uniaxial version of Harts model [5] is cast into the context of ordinary differential equations of first order. An analytical expression for the Jacobian of this ODE-system is given for the solution of the non-linear equation of evolution by means of Newtons method.

The first scheme by Freed & Iskovitz [1] is an explicit/implicit Rosenbrock-Wolfram method. By adding a fifth term to the classical Runge-Kutta method an adaptive algorithm of order 3(4) is derived which is suitable for stiff, non-stiff and even singular differential equations.

The second approach is deduced from a full finite element implementation [2] to handle the same set of equations of evolution as for the first integrator. The key idea for this approach is to approximate the time derivative by a higher order backward difference leading to an implicit equation for the internal variables. A comparison of the solutions of different accuracy leads to an estimate for the local integration error and yields an expression for an optimal time step.

An assessment of benefits and drawbacks of the two methods with regard to their general flexibility in both ODE and FEM-applications is given, for Harts model we use results from literature [4] for a direct comparison.

1. Freed and I. Iskovitz *„Development and Applications of a Rosenbrock integrator"*, NASA Memorandum 4709 (1996)
2. E. Kirchner and B. Simeon *„A higher order time integration method for viscoplasticity"* submitted to Comp. Meth. Appl. Mech. Engng. (1997)
3. E. Hart *„Constitutive relations for the non-elastic deformation of metals"*, Trans. ASME, J. Eng. Mat. Tech. **98**, 193-202 (1976)
4. D. Cordts and F. G. Kollmann *„An implicit time integration scheme for inelastic constitutive equations with internal state variables"*, Int. J. Num. Meth. Engng., **23**, 533-554 (1986)
5. [5] G. Hartmann and F.G. Kollmann *„A computational comparison of the inelastic constitutive models of Hart and Miller"*, Acta Mech., **69**, 139-165 (1987)

Anisotropic Stress/Strain-Rate Relations

Kocks, U.F.
Los Alamos National Laboratory, USA

In 1976, Ed Hart [1] addressed the problem of anisotropy in plasticity and proposed a constitutive relation of the type

$$x_{ij} = (x/X)\, K_{ij;kl}\, X_{kl} \qquad (1)$$

where **x** is an "appropriate strain or strain rate variable" and **X** an "appropriate stress"; when both variables are

chosen deviatoric, the relation invertible. This proposal embodies two insights: that the variables should be *scaled* in an appropriate way; and that the remaining relation between the *directional* quantities should be expressible in tensor form; this is an alternative to expressing them in terms of a plastic potential. We will derive specific relations of this form for a polycrystal made up of crystals that obey a *kinetic* relation between stress and strain-rate. (The limit to a rate-independent material can be easily performed.) In the spirit of Hart's scaling proposal, the macroscopic deviatoric plastic strain rate **D** and the macroscopic deviatoric stress **S** can be decomposed according to

$$\mathbf{D} = \dot{\varepsilon}\,\hat{\mathbf{D}} \qquad \mathbf{S} = \sigma_f\,\hat{\mathbf{S}} \qquad (2)$$

where the scalar $\dot{\varepsilon}$ is truly a time rate of straining, whereas $\hat{\mathbf{D}}$ captures the *straining direction.* σ_f is the 'flow strength' at the reference strain rate $\dot{\varepsilon}$ – a measure of the *scale* of the yield surface or flow potential – and $\hat{\mathbf{S}}$ describes the *shape* of the yield surface. Note that the scalar quantities are *not* the norms of **D** and **S** (as correctly pointed out in [1]); they are, however, defined as work conjugate, so that the scalar product of the directional quantities is identically equal to **1**.

For the purpose of visualization, one may separate the *relation* between stress and strain-rate also into a scalar and a directional one. The first is often represented by a power law (typically *very* nonlinear), and the second can be written like Eq. 1:

$$\hat{\mathbf{D}} = \mathbf{K} : \hat{\mathbf{S}} \qquad (3)$$

The fourth-rank tensor **K** represents the *curvature* of the flow potential: the change of the direction of the normal with a change in the radius vector in stress space. If **K** were constant, Eq.(3) would describe an ellipsoid in stress space. In single crystals and in textured polycrystals, however, the yield surface is faceted and exhibits quasi-vertices. In this case, **K** is a strong function of $\hat{\mathbf{S}}$ and the relations (1) and (3), despite their appearance, are grossly nonlinear. Typically, flow surfaces become less angular the higher the rate sensitivity and the larger the number of deformation modes; this makes 'linear' approximations more likely to be appropriate.

[1] Hart, E.W., J. Eng. Mater. Tech. **98**, 193 (1976).

Flow Stress of FCC Polycrystals with Application to OFHC CU

Nemat-Nasser, S.
University of California at San Diego, USA

Based on the concept of dislocation kinematics and kinetics, paralleled with a systematic experimental investigation, a physically-based model is developed for fcc polycrystals, using OFHC copper for illustration. First, the concept of the motion of dislocations and the barriers that they must overcome in their motion, is used as an underlying *motivation* to obtain general expressions which include a number of free constitutive parameters. These parameters are then evaluated by direct comparison with experimental data.

High-strain-rate compression experiments are performed using the UCSD's recovery Hopkinson technique; see Nemat-Nasser *et al.* (1991, 1994), and Nemat-Nasser and Isaacs (1997). Strains close to 100% are achieved in these tests, over a temperature range of 77 to 1,100K, and strain rates of 10^{-3} to 8,000/s; the quasi-static tests are performed using an Instron machine. For low-temperature tests, both the as-received and annealed samples are tested. Good correlation between the theoretical predictions and experimental results (specially at high strain rates) is obtained with few free constitutive parameters. The orders of magnitude of several of these parameters are first estimated based on the underlying structure of the material. Experimental results are then used to *tune* the final values of these parameters. It turns out that the structure of the constitutive relations and the value of a number of the constitutive parameters are essentially the same for commercially pure tantalum (bcc metal) and OFHC copper. The relation between the two cases is examined and the similarities and differences are discussed.

Nemat-Nasser, S., J.B. Isaacs and J.E. Starrett, "Hopkinson Techniques for Dynamic Recovery Experiments," *Proc. of the Royal Society of London*, A, Vol. 435 (1991), 371-391.

Nemat-Nasser, S., Y.-F. Li and J.B. Isaacs, "Experimental/Computational Evaluation of Flow Stress at High Strain Rates with Application to Adiabatic Shear Banding," *Mechanics of Materials*, Vol. 17 (1994), 111-134.

Nemat-Nasser, S. and J. Isaacs, "Direct Measurement of Isothermal Flow Stress of Metals at Elevated Temperatures and High Strain rates with Application to Ta and Ta-W Alloys," *Acta Materialia*, Vol. 45, No. 3 (1997), 907-919.

Modeling the Development of Residual Stresses In High Strength Steel Arising From Plastic Deformation

Dawson, P. and Boyce, D.
Cornell University, USA

A deformation that may be essentially homogeneous at the macroscopic scale is usually accommodated by the ensemble of constituent crystals in a nonuniform manner owing to the anisotropy of individual crystals and the distribution of their orientations. Such nonuniform deformation over the dimension of a polycrystal leaves the material in an internally stressed condition even after external loads are removed. These residual stresses are an important aspect of the microstructural state of a material following its loading during production. In this paper the development of residual stresses at the level of a

polycrystal is investigated with an elastoplastic polycrystal model and its associated finite element implementation. Sequences of loading and unloading of specimens are simulated, allowing the residual stresses to be computed at several stages in the process of applying a large overall strain. The dependence of the residual stresses on crystallographic orientation is examined by computing the stresses for crystals with particular alignments in relation to the loading direction. Through the use of a scalable parallel implementation, the simulations incorporate thousands of BCC crystals, allowing for accurate estimation of average residual stresses in crystals of the specified orientations. Comparisons are made to values measured by neutron diffraction for a high strength steel alloy.

Session: F1-2 Room: CUB 224 **Time:** M1:30p-3:30p
Chairs: *John Hirth (WSU) & R. Thompson (NIST)*

Crack Arrest in Silicon Single Crystals Leading to Brittle-to-Ductile Transitions in Fracture

Argon, A.S. and Gally, B.
Massachusetts Institute of Technology, USA

Experiments on the arrest of brittle cleavage cracks propagating up a temperature gradient in silicon single crystals will be described and the forms of emission of dislocations from the crack tip, their arrangement on specific planes, and distribution will be discussed and associated with mechanistic models of crack tip stress relaxation. The observations support the importance of the geometrical and energetic conditions for dislocation nucleation from the crack tip even though the final arrest is accomplished after extensive multiplication of dislocations emanating from the initiation sites.

Internal Variable Theory Revisited: Gradient and Stochastic Effects

Aifantis, E.C.
Aristotle University of Thessaloniki, Greek

Internal variables have been introduced into constitutive equations to account for inelastic effects. Among the main contributions in this field, one distinguishes the work of Ed Hart who proposed physically-based internal variable models to describe plastic flow, necking and fracture.

Hart's work provided a new interpretation of internal variables advancing the point of view that they should represent specific microstructural features, with physically motivated evolution equations, rather than being formally introduced as internal parameters which do not enter into the macroscopic work expression. However, heterogeneity aspects and the spatial characterization of internal variables were not included in the above formulation and, thus, phenomena like dislocation patterning and the localization of slip could not be addressed.

The present work revisits the internal variable approach to plastic deformation by considering heterogeneity effects either through the introduction of gradient terms in the deterministic evolution equations or through the stochastic re-formulation of the deterministic evolution equations for the internal variables. Examples include the description and characterization of dislocation heterogeneity during monotonic and cyclic deformation.

Use of Nonproportional and Sequence Experiments to Study the Structure of ISV Constitutive Relations

McDowell, D.L.
Georgia Institute of Technology, USA

Usual tension/compression experiments tend to obscure important first order aspects of material behavior associated with directional hardening and recovery processes. Similarly, combined stress state proportional loading experiments give little information concerning the shape of the flow potential and anisotropy of hardening relations. With regard to viscoplastic constitutive relations, isothermal, constant strain rate experiments do not fully discriminate potentially strong history effects observed in many structural metals. This paper summarizes advances made in understanding the structure of viscoplasticity models for both cyclic loading and finite deformation based on nonproportional loading/straining experiments, sequences of strain rate, and sequences of temperature applied during strain histories on polycrystalline metallics.

Ultra-Small-Angle X-Ray Scattering by Single Crystal Al Deformed In-Situ

Levine, L.E. and Long, G.G., Thomson, R.M.
National Institute of Standards and Technology, USA

Among the earliest small-angle x-ray scattering and small-angle neutron scattering experiments were attempts to study dislocation structures. These structures have proven to be very difficult to measure because of the intrinsically low contrast of the microstructure, the strong angular dependence of dislocation scattering, and the requirement that multiple Bragg diffraction be strictly avoided. Thus, many attempts to measure dislocation structures have been compromised by these difficulties. The current series of experiments are the first results to map out the detailed behavior of scattering by dislocations and dislocation structures. A collimated, monochromatic, long-wavelength X-ray beam passes through a 150 micro-meter thick aluminum single-crystal and the USAXS is measured as a function of applied stress and plastic strain. As the crystal is deformed by uniaxial

tension, dislocation walls develop. The scattered intensity is observed to be power-law and depends strongly on the dislocation density, the dislocation structure, and the sample/beam geometry.

Interpretation of these experimental results has required the development of a new theory of small-angle scattering from dislocation structures. All of the observed USAXS features are readily interpreted using this theory. A particularly important result is the prediction that only a well defined sub-set of dislocations satisfying strict geometrical rules will be visible in a USAXS experiment. This allows experiments to be designed that can follow the evolution of selected subsets of dislocations within a deforming metal sample.

Consideration of Processes on the Microscale and Mesoscale for the Development of Constitutive Models for Metallic Materials

Steck, E.A.
Technische Universität Carolo-Wilhelmina zu Braunschweig, Germany

Processes on the microscale determine the macroscopic behaviour of metallic materials and should therefore be considered during the development of constitutive macroscopic equations used for engineering calculations. The paper reviews the mathematical formulation of the most significant of these processes, such as dislocation motion due to thermal and mechanical activation and the development of internal structures during plastic deformation. It describes the consideration of these relations in a stochastic model for the inelastic behaviour of metals and shows the comparison between predictions of this model and experimental findings. Most engineering materials possess a polycrystalline structure. Under load, the anisotropy of the constituent grains causes strong inhomogeneities of stresses and strains between and inside the grains. Especially strain localisations are of great importance because they are possible starting points for damage. In order to investigate these local deformation processes, a model based on the Finite-Element-Method is introduced. The main purpose of the model is to investigate the local deformation behaviour of polycrystals on the grain level. Numerical simulations of local plastic flow in polycrystals are in good agreement with the results of metal physics and experiments.

Session: F1-3 Room: CUB 232 **Time:** T9:30a-11:30a
Chairs: *A. Khan (U. Maryland)*

On Non-Proportional Multi-Axial Experiments in Plasticity

Khan, A.S.
University of Maryland Baltimore County, USA

Several non-proportional multi-axial experiments and their limitations will be discussed including tension followed by torsion and vice-versa, chanel-die and compression in presence of confining pressure. Experimental results on 1100-0 Aluminum, OFHC Copper, tantalum and tantalum alloys, will be presented and discussed in relation to the predictions of various constitutive models.

On the Mechanics of the Heart

Onat, E.T.,
Yale University, USA

The left ventricle of (mammalian) heart has been the subject of extensive studies. Thanks to new imaging techniques increasingly detailed and quantitative knowledge is becoming available on the fields of displacement and deformation in the ventricle muscle over a cycle of pumping. Interpretation of these observations requires the use of realistic, yet tractable representations of mechanical behavior of healthy or diseased parts of the heart muscle. The paper summarizes some incipient collaborative efforts in this direction.

The starting point of our work is the simple, but rather unrealistic, case where the shape changes and rotations are small and blood flow and viscosity within the muscle are ignored. We assume that the total strain $\varepsilon(\mathbf{x}, t)$ at the location $\mathbf{x}$ and time t is composed of the live strain $\varepsilon^{L}(\mathbf{x}, t)$ created by the heart muscle and of the strain $\varepsilon^{\sigma}(\mathbf{x}, t)$ caused by the Cauchy stress $\sigma(\mathbf{x},t)$:

$$\varepsilon(\mathbf{x}, t)\ \varepsilon^{L}(\mathbf{x}, t) + \varepsilon^{\sigma}(\mathbf{x}, t)$$

$$\varepsilon^{\sigma}(\mathbf{x}, t) = \mathbf{D}(\mathbf{x})\ \sigma(\mathbf{x}, t)$$

where $\mathbf{D}(\mathbf{x})$ is the elastic compliance of the heart muscle.

The pumping action of the ventricle is the result of the ion induced contractions of myocytes. These contractions produce local shape changes described by $\varepsilon^{L}(\mathbf{x}, t)$.The muscle elements also change shape under the stress field $\sigma(\mathbf{x}, t)$ created by the blood pressure in the ventricle cavity. It is reasonable to expect that, in the absence of stresses, the deformed elements would fit together, without leaving fissures, to form the global deformed shape of the ventricle. Thus it would be a good starting hypothesis to assume that the field of live strains $\varepsilon^{L}(\mathbf{x}, t)$ is compatible.

As an illustration of these ideas we consider and calculate the living strains that should be produced by a "cylindrical heart" in order to maintain a "measured" pressure - volume cycle.

One of the aims of our work is to study the additional stresses that will be caused by the non compatible changes in $\varepsilon^{L}(x, t)$ resulting from a decrease of blood supply in an infracted region of the heart.

Hardening and Strain Localization in Ductile Crystals

Bassani, J.L.
University of Pennsylvania, USA

Within the setting of continuum theory where slips (shears) on crystallographically-defined systems provide the kinematical mechanisms for plastic flow, we have shown that fine secondary slips contribute significantly to overall hardening behavior and also play an important role in the nucleation and stabilization of localized modes of deformation. Localized, patterned deformation is widely observed during plastic flow of single- and poly-crystalline metals as well as metal-matrix composites. One prominent example is the evolution of coarse slip bands in ductile single crystals. This lecture focuses on constitutive relations for multiple-slip hardening and an analysis of coarse slip.

State Variable Constitutive Modeling Using Physically Based State Variables

Field, D.P.
TexSEM Laboratories, USA

Since the early spring and dash-pot constitutive models of Hart three decades ago, numerous state variable models have been proposed to describe the behavior of materials. Some of these models have been remarkably successful in predicting material response over a limited domain, while others are somewhat less successful, but are capable of modeling material behavior over a wide range of conditions. Virtually all state variables are described from the foundation of observed phenomenology of the modeled processes, but are not based upon physically measurable features of the microstructure. Constitutive models which incorporate descriptions of physically measurable microstructural entities as state variables offer a distinct advantage over phenomenological models. This advantage lies in the inherent potential of physics based models for predictive capability and use in alloy design, assuming evolution equations are sufficiently based upon physical principles. Since dislocation structure development generally controls hardening behavior of crystalline materials, a suitable mathematical description of these structures for use in modeling is required. Historically these structures are reduced to simple measures of dislocation density or cell size for use in models. Researchers that attempt to describe the evolution of dislocation cell morphology on a more detailed level offer qualitative descriptions which aid in understanding cell development, but cannot be directly included in modeling efforts.

A physically measurable state variable for an idealized material containing hard particles in a soft matrix could be merely the volume fraction of hard particles. It may be more realistic, however, to include the statistics of the size and shape distributions of particles and their spatial arrangement as significant clustering will obviously change the observed behavior. Various such microstructures are considered in the present work and the procedure to identify the variables with first order effects are outlined.

Finally, a particle free commercial purity aluminum material is analyzed with various measures of the microstructure considered as state variables. The dislocation cell structure morphology as a function of the local and neighboring crystallite lattice orientations is determined to be the controlling variable under the imposed deformation conditions. A model form is proposed which describes the constitutive behavior of such alloys.

Relaxation Behavior and Constitutive Modeling

Krempl, E.
Rensselaer Polytechnic Institute, USA

In the 1970s E. W. Hart pioneered the relaxation test for determining inelastic material behavior data. Performing relaxation tests (zero total strain rate is required) at that time was difficult (servo-hydraulic, strain-controlled testing and strain measurement on the gage length became available after these investigations). Data obtained from "hard" testing machines had to be converted via formulae derived in the theory of the tensile test. A scaling law of the log stress versus log inelastic strain rate curves that led to one master curve was derived. All data were generated using repeated loading and intermittent relaxation periods with one loading strain rate.

Recently, the viscoplasticity theory based on overstress (VBO) was developed by the author and his students. In VBO only elastic and inelastic strain rates are considered. The inelastic strain rate can be a function of the overstress, the difference between the stress and the equilibrium stress that is a state variable of the theory. For constant strain rate tests VBO admits long-term solutions that render the overstress constant for any constant slope. This solution is thought to apply in regions where plastic flow is fully established. According to VBO relaxation tests started in the regions of fully established plastic flow should exhibit relaxation curves that can be made coincident by a shift along the stress axis. Using this property of VBO it is easy to show that the stress-inelastic strain rate curves should coincide upon a shift along the stress axis. This has been demonstrated using published data by Hart and collaborators.

Tests with different constant strain rates, some interrupted by relaxation periods, all of equal duration were performed on several alloys and Nylon 66 with the following results:

For a given prior strain rate and for a constant relaxation time the stress drop can be nearly independent of the stress or strain at which relaxation starts.

However, the stress drops for constant relaxation times depend strongly on the strain rate preceding the relaxation tests. They increase with an increase of prior strain rates.

The increase with prior strain rate is nonlinear (Increasing the prior strain rate by a factor of ten increases the stress drop in a given relaxation time by far less than a factor of ten).

At the end of the relaxation periods the test associated with the fastest (slowest) prior strain rate has the smallest (largest) stress magnitude.

The ramifications of these and other observations regarding relaxation behavior are discussed and it is shown that VBO has no difficulty in reproducing these newly found phenomena.

Session: F1-4 **Room:** CUB 232 **Time:** T1:00p-3:00p
Chairs: *O. Onat (Yale U.) & H. Garmestani (FSU)*

Thermodynamic Description of Fracture In Inelastic Materials. Similarity With Phase Transitions

Levitas, V.I.
University of Hannover, Germany

Fracture is treated as a thermomechanical process of decrease of elastic moduli in some region from the initial value to zero which is accompanied by a decrease in yield stress, i.e. as a special second order phase transitions. Recently developed thermomechanical theory of martensitic phase transitions in inelastic materials [1, 2] is reformulated for the fracture problem. Using the second law of thermodynamics, the driving force for fracture is derived as the dissipation increment in the fractured region during the whole fracture process and due to fracture only (i.e. total dissipation increment minus plastic dissipation increment). Temperature variation is taken into account. Fracture in the given volume will occur when calculated driving force reaches its experimentally determined value. Using the postulate of realizability [1 - 3], the extremum principle for the determination of all unknown parameters (e.g. shape and dimension of fracture region or direction of crack propagation) is derived. It is shown that for the fracture in elastic materials the proposed approach gives alternative but equivalent to the principle of minimum of Gibbs energy formulation and known classical results. Thermodynamical consistent kinetic equation for fracture is derived for time dependent processes. Some aspects of the formulation of boundary—value problem are analyzed. Some possible ways of formulation of constitutive relations for inelastic deformations in the course of the fracture are discussed.

1. Levitas, V. I. (1997) Phase transitions in elastoplastic materials: continuum thermomechanical theory and examples of control. Part I and II. J. Mech. Phys. Solids, vol. 45, 923--947 and 1203--1222.
2. Levitas, V. I. (1998) Thermomechanical theory of martensitic phase transformations in inelastic materials. Int. J. Sol. Structures, vol. 35, 889--940.
3. Levitas, V. I. (1995) The postulate of realizability: formulation and applications to post—bifurcation behaviour and phase transitions in elastoplastic materials. Part I and II. Int. J. Eng. Sci., vol. 33, 921--971.

Influence of Stacking Fault Energy, Grain Size, and Stress State on Deformation Twinning in fcc Polycrystals

Kalidindi, S. R., El-Danaf, E. and Doherty, R.D.
Drexel University

This paper investigates the microstructural variables influencing the stress required to produce deformation twins in polycrystalline face-centered cubic (FCC) metals. Classical studies on FCC single crystals have concluded that the deformation twinning stress has a parabolic dependence on the stacking fault energy of the metal. In this paper, new data is presented indicating that stacking fault energy has only an indirect effect on the twinning stress. The results indicate that the *dislocation density* and the *homogeneous slip-length* are the most relevant microstructural variables that influence directly the twinning stress in the polycrystal. The role of the stacking fault energy was observed to be critical in building the necessary dislocation density while maintaining relatively large homogeneous slip-lengths. It was also observed that the stress state (e.g. simple compression, plane strain compression, simple shear) has an important influence on both the strain hardening rates and the microstructure evolution in the low SFE polycrystals. These results will be presented and discussed.

A General Representation of a Titanium Alloy Capturing Reversible and Irreversible Hereditary Behavior

Arnold, S.M., Saleeb, A.F. and Castelli, M.G.
NASA Lewis Research Center, USA

A Micromechanical Model for Metal Creep

Shih, W.Y.
Texas Instruments, Inc., USA

A micro-mechanical model proposed by Hart is extended and analyzed. The model has a distribution of cell structures in every crystal grain. Each cell is a volume of low defect density. The cell wall that separates two neighboring cells is regarded as a relatively dense array of dislocations.

A representative cell is bounded by two infinite, straight cell walls consisting of identical edge dislocations. Upon the application of an *applied shear stress*, a band of gliding edge dislocations develops in a glide plane. The cell wall dislocations, which are allowed only to climb, block the glide dislocations from moving out of the cell. The glide band is held in quasi-static equilibrium; and the stability of the cell is thus maintained. In turn, a climb force field is generated by the glide band which drives the wall dislocations away from the cell wall—glide plane intersection.

To avoid unnecessary complications, dislocation glide in the glide plane is assumed to be frictionless; and linear kinetics is employed to relate the climb velocity to the climb force on wall dislocations. Under a remotely applied *shear stress*, the time evolution of the discrete cell wall dislocations and the equilibrium positions of the glide band tip are numerically simulated. The wall dislocations climb {\em away} from the cell wall—glide plane junctures due primarily to the climb force produced by the glide band. When the equilibrium of the glide band tip becomes unstable as a result of such climb motion, the lead glide dislocation is injected into the cell wall. A new cycle of climb and injection then start over again. The rate of such injections, which accounts for most of the inelastic strain rate, varies slowly at a fixed applied stress. This approach of simulation is limited by the finite number of cell wall dislocations that can be monitored in the digital computation and fails when the applied stress becomes sufficiently small.

A continuum model is then formulated which retains the key features of the discrete one. It avoids the finite—size effect in the discrete—dislocation simulation and extends the stress range to lower levels. Numerical solutions for the injection rates at various values of the *applied stress* provide a good fit to the experimental behavior obtained by Hart and others.

Phenomenological Modeling of Transient Behavior in Cyclic Loading and Relaxation

Garmestani, H. and Hart, E.W.
FAMU-FSU College of Engineering, USA

Hart proposed a unified state variable model which has been shown to be capable of predicting the nonelastic deformation for low and high temperatures over a very large strain rate range(1). Hart's constitutive equations are relations among the applied stress deviator σ, the observable non-elastic strain rate $\dot{\varepsilon}$, and two state variables - a tensorial internal state variable **a**, and a scalar state variable σ^*, called the hardness parameter (or the isotropic hardening parameter). He developed the form of these relations from experimental evidence and a heuristic consideration of micro-mechanism in polycrystalline materials (1, 2). Some of the important parameters can be uniquely determined using load relaxation tests in the fully loaded regime. The model was based on the realization that the dislocation motion is limited by the dislocation glide friction and by the resistance to strong barriers represented by the hardness parameter σ^*. The passage of dislocations through strong barriers results in unrecoverable plastic deformation and the resistance to dislocation motion produces an anelastic strain (internal stress) due to pile-up of dislocation. It was proposed that the glide of dislocations occurs by a viscous process and that is the basis for the apparent hysteresis and transient phenomena. A simple power law relationship for the frictional glide stress was used to define the steady state condition of the transient process. The interaction of the viscous process at non-steady conditions and the internal stress was the basis for such behaviors as cyclic loading, reloading phenomena, and the Bauschinger effect.

A transient model based on non-steady state condition for the frictional glide process is introduced here using a transient stress as a new state variable. The evolution of this variable is very similar to that proposed for the hardness parameter except that the recovery parameter plays a major role. The power law relationship for the frictional glide process is a steady state condition for the transient behavior in this model. The results show that the model can predict the transient behavior for both cyclic loading and the reloading phenomena during plastic deformation and load relaxation .

1. E. W. Hart, *J. Eng. Mats. & Tech.* **98**, 193-202 (1976).
2. E. W. Hart, *Journal of Engineering Materials and Technology* **106**, 322-325 (1984).

Symposium F2
Multi-Scale Modeling of Deformation and Fracture
Organizers
R. Thomson
National Institute of Standards and Technology, USA
J.P. Hirth & H.M. Zbib
Washington State University, USA

Session: F2-1 Room: Cascade 123 **Time:** M10:00a-12:00p
Chairs: *T. D. de La Rubia (LLNL) & S. J. Zhou (LANL)*

Atomistic Finite Deformation Simulations

Horstemeyer, M.F. and Baskes, M.I.
Sandia National Laboratories, USA

Finite deformation plasticity models have been developed from a top-down approach in length scales. Unified-creep-plasticity models, internal state variable models, and crystal plasticity models are such examples that have experienced some success in solving boundary value problems in the context of finite element simulations. They have also been used to give insight and understanding of various features such as the plastic spin, plastic rate of deformation, texture, failure, etc. To date, finite deformation plasticity has not been thoroughly examined at the atomistic scale. In this paper, we present results for single crystal Nickel that has undergone compression and simple shear loading up to 30% effective strain. In this bottom-up approach, we motivate physical mechanisms for top-down plasticity constitutive models. In particular, we analyze the distribution of deformation gradient, velocity gradient, stress state, misorientations, and microtexture that occurs within the highly heterogeneous single grain. In order to bridge length scales, we believe that a systematic method of determining hardening mechanisms from a bottom-up approach is key. As such, we lay out a plan for determining these key length scale links using atomistic simulations.

This work was supported Sandia National Laboratories by the U. S. DOE under contract no. DE-AC04-94AL8500

Atomistic Simulations for Multiscale Modeling in bcc Metals*

Moriarty, J.A., Xu, W., Söderlind, P., Belak, J.F., Zhu, J. and Yang, L.H.
Lawrence Livermore National Laboratory, USA

Multiscale modeling of plastic flow and other mechanical properties in bcc transition metals requires an accurate atomistic description of deformation and defect energetics as input into larger length scale simulations such as 3D dislocation dynamics at the microscale. We are using state-of-the-art electronic-structure and interatomic-potential methods to study a wide range of fundamental properties of bcc metals, including elastic moduli, ideal shear strength, the atomic structure and energetics of vacancies, dislocations, and grain boundaries, and dislocation-dislocation interactions. The current focus of this work is on the prototype metal tantalum (Ta), where mechanical behavior at both ambient and extreme conditions is being addressed. A comprehensive set of *ab initio* electronic-structure calculations have been performed in the 0-10 Mbar pressure range in Ta [1] and used together with rigorous generalized pseudopotential theory (GPT) to develop corresponding model-GPT (MGPT) multi-ion interatomic potentials [2] suitable for realistic atomistic simulations. Many-body angular forces, which are accounted for in the MGPT through explicit three- and four-ion potentials, are generally important to the structural and mechanical properties of bcc transition metals. In this regard, selected grain boundary structures have been calculated for comparison with concurrent HREM measurements, as an additional validation test for the Ta MGPT potentials. With regard to dislocations, our previous studies on Mo [3] have now been extended to Ta and generalized in scope. In the present work, we have investigated the core structure, the gamma surfaces, and the Peierls stress and related energetic barriers associated with the motion of <111> screw dislocations on the primary {110} and {112} slip planes in this metal. In addition, we are calculating kink-pair formation, migration, and activation energies, including both their stress and orientation dependence. These latter quantities control the low-temperature plasticity in bcc metals and are essential input for microscale dislocation-dynamics simulations. We are also studying dislocation-dislocation interactions in an attempt to accurately model junction formation and breaking, which are fundamental to the description of strain hardening at the microscale. In the future, we hope to perform dynamic simulations of dislocation mobility and dislocation-dislocation interactions using accelerated molecular dynamics schemes on massively parallel computers. Advanced parallel versions of our static dislocation simulation codes are also being developed.

[1] P. Söderlind and J. A. Moriarty, Phys. Rev. B (1998, in press).
[2] J. A. Moriarty, Phys. Rev. B **49**, 12431 (1994) and **42**, 1609 (1990).
[3] W. Xu and J. A. Moriarty, Phys. Rev. B **54**, 6941 (1996) and Comput. Mater. Sci. (1997, in press).

*This work has been performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

Atomistic Simulations of Dislocation Intersection Process - A Step to Bridge Approaches Across Length Scale

Zhou, S.J. and Preston, D.L.
Los Alamos National Laboratory, USA

Deformation of metals and intermetallics is closely related to dislocations and their interactions. One of important questions is how a dislocation moves through a dislocation forest, which is one of the important mechanisms restricting the dislocation motion and contributing to work hardening. In this meeting, we will report our study on the perpendicular intersection process of extended dislocation in single-crystal copper with 3D molecular dynamics simulations with up to 3.5 million atoms at very low temperature.

The intersection process, which involves three of the four possible {111} glide planes in the face-centered cubic lattice, begins with junction formation, followed by unzipping, partial dislocation bowing, cutting, and finally unit jog formation. The critical stress estimated from the measured breaking angle, 70^0, is in good agreement with the value measured from MD simulations. It is interesting to note that the jog line on the mixed dislocation is not contracted and deviates from <011> to <112> directions without creating vacancies or interstitials (*i.e.* conservative motion). However, the jog on the screw is fully contracted, or nearly so. This investigation provides insights into these complex atomistic processes, which are currently not accessible to experimental investigation and are essential to macro/meso-level deformation modellings.

Molecular Dynamics Simulations of Dislocation-Defect Interactions and Microstructure Evolution in Irradiated Metals*

de la Rubia, T.D., Alonso, E.A. and Shastry, V.
Lawrence Livermore National Laboratory, Livermore, USA

Modeling microstructure evolution in irradiated materials requires a good understanding of the interaction between the induced defect populations and the dislocations present in the material. In this paper we discuss a hierarchy of simulation tools that describes defect production and damage accumulation in irradiated metals over macroscopic length and time scales. First, we describe how defects are produced in the form of small vacancy and interstitial dislocation loops and discuss simulations of the energetics and mobilities of these small loops. In addition, we present the results of molecular dynamics simulations of the interaction between self interstitials, vacancies and small prismatic interstitial loops with dislocations. These studies are carried out by coupling the atomistic simulations to an infinite elastic continuum using flexible boundary conditions and lattice Green's functions. These results are then used as input to a kinetic Monte Carlo (KMC) simulation of defect diffusion, clustering and accumulation in the lattice. The KMC simulations provide information on the rate of accumulation of interstitial loops at network dislocations, the rate of growth of vacancies voids, and the rate of impurity diffusion and precipitation. The results are compared to available experimental data and discussed in the context of existing and new models of radiation-induced microstructure evolution, hardening and void swelling.

*This work was performed by Lawrence Livermore National Laboratory under the auspices of the US Department of Energy under contract W-7405-Eng-48.

Elastic Interactions of Defects on Crystal Surfaces

Kouris, D., Peralta, A., Knap, J. and Sieradzki, K.
Arizona State University, USA

Surface defects corresponding to atoms, vacancies, and steps interact with one another affecting and often dominating kinetic processes associated with thin-film growth. It is now well recognized that the primary interaction among these defects is through their elastic fields. A harmonic lattice model for an adatom at the (001) surface of a cubic crystal is developed, based on the concept of eigenstrains. The eigenstrains introduced by the adatom are obtained directly using EAM potentials. This formulation includes both in-plane and out of plane distortions. The elastic field of the adatom is described and the limitations of the continuum theory are discussed. In this scheme, the model of a surface step is a natural consequence of an appropriate aggregate of adatoms. Calculations of the interaction energy between adatoms, steps, and adatoms and steps indicate agreement with existing, long-range results. It was found that anisotropy plays a significant role in this process. For example, in certain crystallographic directions, identical adatoms attract each other. Independent simulations using EAM potentials clearly demonstrate the accuracy of the elastic field produced by the eigenstrain model. As a result, the restrictive assumptions regarding the adatom/force system found in existing models are removed in this distortion-based model.

Session: F2-2 Room: Cascade 123 **Time:** M1:30p-3:30p
Chairs: *N. M. Ghoniem (UCLA) & H. Huang (LLNL)*

Interaction between Curved Dislocation Segments in 3-D Dislocation Dynamics

Ghoniem, N.M. and Baccaloni, M.
University of California Los Angeles, USA

The long-range interaction between dislocation segments is a major ingredient in the simulation of plastic deformation of materials via the methodology of Dislocation Dynamics. Since the stress field of dislocations falls off as the inverse of the distance from the dislocation, it is of a long-range nature. For a collection (N) of interacting dislocations, this would lead to N^2 calculations for every time step of a dynamical simulation. Therefore, the computational burden becomes prohibitively large when N is large. Current methods of stress calculations are generally based on the interaction between straight segments. Hence, heavy linear segmentation is required to represent curved dislocations, with an associated computational penalty. In this work, we present a method for calculating the components of the elastic field of curved segments, without any special constraints. The elastic field tensors (e.g. stress, strain, etc.) can thus be computed for an arbitrarily curved segment, and then the interaction forces, mutual inductance and energetics can be recovered. The method is based on the work of both Kroner and De Wit, with the present extension introducing a parametric representation of dislocation loops in 3-D vector fields. Results of the calculations will be compared to known cases, and the computational gain assessed in this work.

Study of Frank-Read Sources Within a Continuum Simulation

Chrzan, D.C.
University of California, Berkeley, USA

A continuum simulation of dislocation dynamics has been developed and used to study the dynamics of Frank-Read sources. The simulation is based on isotropic elasticity theory, and includes the self-stress of the dislocations, as well as dislocation/dislocation interactions. The equations of motion are integrated using a variable step, fourth-order Runge-Kutta integration routine coupled with a dynamic gridding algorithm. The algorithm is very stable, and introduces minimal noise into the observed dislocation structures. The technique can be used to model approximately 10^{-4} m of dislocation using a desktop workstation. As such, the technique is best suited for studying the details of interactions between a small number of dislocations.

The simulations have been applied to the study of two aspects of Frank-Read source operation. First, the critical stress needed for operation of Frank-Read source was calculated using the dynamics simulations. The algorithm predicts results consistent with the results expected from approximate analytical treatments, and this serves as a verification of the accuracy of the stress calculation. The dynamics of Frank-Read source operation form the second aspect studied. Simulation of dislocation dynamics requires a mathematical statement of the relationship between the net stress felt by a dislocation segment, and the subsequent velocity of that segment. Though central to all simulations of this type, relatively little is known about this relationship. In the current study, the velocity is *assumed* to be proportional to the mth power of the net force felt by a segment, where m is chosen to be either 1 or 3. The area swept out as a function of time by a source is studied as a function of applied stress. It is found that for both choices of m, the area displays an approximate t^3 dependence on the operation time. In addition, it is demonstrated that sources operating just above their critical stress for operation may display transient behavior extended over many orders of magnitude in time. The temporal extent of this transient is observed to increase with m. Though unlikely to be of significance for creep experiments, this delay time may have ramifications for modeling dislocation multiplication mechanisms at a continuum mechanics scale.

This research is supported at Lawrence Berkeley Laboratories, Materials Science Division through the Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division, U. S. Department of Energy, under Contract No. DE-AC03-76SF00098.

Dislocation Dynamics from Kröner to Simulations & a Proposed New Dynamical Treatment

El-Azab, A.A.
University of California, Los Angeles, USA

Plastic deformation of metals has been a fascinating research topic for metallurgists, solid mechanicians, physicists and mathematicians for over a century. Amazingly though, these communities are still searching for answers to numerous questions related to such a phenomenon. The elegant theory of continuum dislocations was founded about half a century ago, and has been set aside for a number of decades. Theoretical development of this theory were advanced to treat dynamical problems as well. These developments, however, were undertaken in such a manner which rendered the theory limited to internal stress field calculations, as the pertinent tensorial dislocation densities and fluxes were considered as input. In the context of plastic deformation, however, these densities and fluxes represent fundamental output from which deformation fields should be derived under the action of external loads. Limited attempts were made to evolve this theory in this direction and the

rigor and elegance of the theory were not of significant use.

During the past decade or so, results on plastic deformation using brute force computer simulations of the dynamics of dislocation ensembles started to appear. Unfortunately, though, such computer-based models are still suffering from inconsistencies related to unrealistic phenomenological input, sever computational errors of the long-range stress fields, and violation of the primary requisites of real dislocation microstructures.

In the present communication, we briefly review the classic developments of the theory of dislocated crystals, both static and dynamics, and extract a version of the theory which is suited for discrete computer simulations. Additionally, we present an outline of extension of the classic theory to treat tensorial dislocation densities and fluxes as output of the theory, thus evolving the theory as a tool to predict plastic deformation fields, both homogeneous and localized. The essential features of these modifications are based on relating the internal fields to the dislocation fluxes, including short-range interactions and cross slip in a continuum fashion, preserving the three-dimensional and discreteness character of the deformation process, and coupling to various thermally activated processes in the dislocated crystal. Since the present work is still under development, only preliminary results may be available at the time of this conference.

Stability of Dislocation Short-Range Reactions in BCC Crystals

Huang, H.
Lawrence Livermore National Laboratory, USA
Ghoniem, N.M.
University of California, Los Angeles, USA
de la Rubia, T.D.
Lawrence Livermore National Laboratory, USA
Rhee, M., Zbib, H.M. and Hirth, J.P.
Washington State University, USA

The stability of short-range reactions between two dislocations of parallel line vectors which glide on two parallel slip planes in BCC crystals is determined. The two dislocations are assumed to be infinitely long, and their interaction is treated as elastic. The interaction and self-energies are both computed for dynamically moving dislocations, where the dependence on dislocation velocity is taken into account. The stability of the reaction is determined as a function of the following phase space variables: relative angle, relative speed, dislocation mobility, Burgers vector, separation of slip planes, and external force. It is found that the dynamic formation of dislocation dipoles or tile wall embryos occurs only over a small range of the investigated phase space. Inertial effects are shown to be important at close separation, because of the large force between the two dislocations comprising the dipole or tilt wall embryo. Destabilization of the dislocation dipoles or tilt wall embryos is found to be enhanced by externally applied stresses or by stress fields of neighboring dislocations.

Models For Long/Short Range Interactions and Cross slip In 3D Dislocation Simulation of BCC Single Crystals

Rhee, M., Zbib, H.M. and Hirth, J.P.
Washington State University, USA
Huang, H. and de la Rubia, T.D.
Lawrence Livermore National Laboratory, USA

Models and rules for short range interactions, cross slip and long range interactions of dislocation segments for implementation into a 3D dislocation dynamics (3DD) model are developed. Dislocation curves of arbitrary shapes are discretized into sets of straight segments of mixed-dislocations. Long range interactions are evaluated explicitly based on results from the theory of dislocations. Models for short range interactions, including, annihilation, formation of jogs, junctions, and dipoles are developed on the basis of a "critical-force" criterion that captures the effect of the local fields from surrounding dislocations. Also a model for the cross slip mechanism is developed and coupled with a Monte-Carlo type analysis to simulate the development of double cross-slip and composite slip. The model is then used to simulate stage I (easy glide) stress-strain behavior in bcc single crystals, illustrating the feasibility of the 3DD model in predicting macroscopic properties such as flow stress and hardening, and their dependence on microscopic parameters such as dislocation mobility, dislocation structure, and pinning points.

Session: F2-3 Room: Cascade 123 **Time:** M4:00p-6:00p
Chairs: *D. Lassila (LLNL) & W. King (LLNL)*

Time-Resolved Response of Shocked Materials at Different Length Scales

Gupta, Y.
Washington State University, USA

Experimental Investigations of Size Effects of FCC Polycrystal by Shear Banding

Watanabe, O. and Kurata, T.
University of Tsukuba, Japan

Several plasticity phenomena display a size effect where the smaller the size is the stronger its response. In the deformation of polycrystal, the mismatch of slip at the boundaries of the grains may include gradients of plastic strain, as is discussed previously. This paper contains a report of an experimental meso-scale study using FCC polycrystal of pure Aluminum and OFHC

Copper in both of tension and compression loading. Experimental measurements are carried out to investigate thickness effects and grain size effects together with geometrical size effects. The geometrical size effect is tested by changing its geometrical sizes of cross sectional area from 1x2 mm enlarging similarly to 6x12 mm every 1 mm. The thickness effect is tested by changing its thickness from 1 mm to 6 mm with the width of cross section of 12 mm constant, and grain size effect is tested by changing heat treatment for OFHC Copper to produce about three times larger grain in diameter. It may be concluded from the stress-strain curves that material response becomes stiffener for smaller, thinner and finer-grain specimens. SES observation can clarify the internal mechanism of plastic flow in the specimens. The direction of micro shear band may change or the slip itself stops at the grain boundaries, and double-slip may occur in free edge surface. The cut-off surfaces show the typical ductile and shearing fracture processes for large and small specimens, respectively, which relates to the size effects appeared in stress-strain curve. Phenomena dominant of shear deformation process may produce strain gradient, leading to size effect. Continuum 3-dimensional FEM analysis and crystal plasticity analysis using Voronoi tessellation also indicate that sharp shear banding may easily occur in smaller, or thinner size specimens.

Experimental Study of Internal Variable Evolution in 304L Stainless Steel at Multiple Strain Rates and Temperatures

Harley, E.J. and Miller, M.P.
Cornell University, USA, and
Bammann D.J.
Sandia National Labs, USA

Most metals exhibit a deformation-induced uniaxial yield strength asymmetry commonly referred to as the Bauschinger effect. Interpreted within the context of macroscale viscoplastic models, it is conventional to describe this yield strength asymmetry with two internal hardening variables. They are typically referred to as the scalar, isotropic hardening, kappa, and the tensorial, kinematic hardening, alpha. The focus of this work was to conduct a series of reverse yield experiments to measure the evolution of these two hardening components in 304L stainless steel (SS304L) over a range of temperatures and strain rates. In this paper we discuss how to determine the magnitude of alpha and kappa from the experimental data and then to subsequently integrate the evolution equations to determine a set of model parameters. In a rate-dependent viscoplastic model, strain rate dependence can be placed directly in the flow rule, in the evolution equations, or both. A methodology for partitioning the rate and temperature dependence between the flow rule and the evolution of alpha and kappa is presented.

All reverse yield experiments were conducted on fully-annealed SS304L at true strain rates of 10-2 s-1 and 10-4 s-1, temperatures from 20oC to 1000oC, and prestrain levels up to 13.5% or 30%, depending on temperature. One consistent result obtained from these experiments was that, when employing a 50 ustrain offset definition of yield, the magnitude of alpha increases from 0 MPa to a significant percentage of the flow stress within the first 0.5% of plastic strain at all temperatures and strain rates. To gain further insight into the strain rate and temperature dependence of the mechanical behavior of this material, strain rate jump experiments and stress relaxation experiments were performed at each rate and temperature. SS304L is a metallurgically complicated material with multiple deformation mechanisms operating over a broad range of length and size scales. For instance, some of the strain hardening character of SS304L is determined by twinning and dislocation structures on one scale and solute diffusion on another. Hence, we observed serrated yielding associated with the Portevin-Le Chatelier effect at 650 C. The details of individual processes operating at the microstructural level are not clearly resolved at the macroscopic level we observed them. Therefore, one may question whether a representation with two macroscopic internal variables can accurately capture the behavior of this material over such a broad temperature regime. In this paper, therefore, we examine the consistency of the rate and temperature dependence we experimentally observed in the evolution of alpha and kappa with the representation of the kinetics in their evolution equations.

Mechanical Behavior of Ta and Ta-W Alloys and Their Associated Dislocation Structures

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A wide range of mechanical testing was performed on numerous annealed tantalum and tantalum-tungsten alloy plate materials. These tests included uniaxial testing in compression at strain rates of 10-3 s-1 and 3000 s-1 and at temperatures of 77 or 300K. In general the Ta-W alloys exhibited greater work-hardening behavior. Extensive transmission electron microscopy study of annealed and deformed materials indicated that the annealed samples had a significant dislocation density in some areas of the sample and this density increased with increasing tungsten content. Also, at a given value of plastic strain the dislocation density increased with additions of tungsten, as well as increasing strain rate and decreasing test temperature. This significant effect of W alloying additions on stress-strain response and dislocation character will be discussed in terms of its effect on the athermal

component of flow stress and the ease of kink migration.

Orientation Imaging Microscopy Investigation of the Compression Deformation of a [110] Ta Single Crystal

Schwartz, A.J., King, W.E., Campbell, G.H., Lassila, D.H., Sam, D.S. and Shu, J.Y.
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High-purity tantalum single crystal cylinders oriented with [110] parallel to the cylinder axis were deformed 10, 20, 30, and 40 percent in compression. The samples take on an ellipsoidal shape, elongated along the [001] direction with almost no dimensional change along $[1\bar{1}0]$. The samples were subsequently sectioned for characterization using Orientation Imaging Microscopy (OIM). OIM reveals the crystal rotations that arise from the accumulation of geometrically necessary dislocations. Two orthogonal sectioning planes were selected: one in the plane containing [001] and [110] (longitudinal) and the other in the plane containing $[1\bar{1}0]$ and [110] (transverse).

To examine local lattice rotations, the Euler angles relative to a reference angle at the section center were decomposed to their in-plane and out-of-plane components. The in-plane and out-of-plane misorientation maps for all four compression tests reveal inhomogeneous deformation everywhere and particularly large lattice rotations in the corners of the longitudinal section. In the longitudinal plane, rather sharp changes in crystal orientation (~1°) are observed that appear to be geometric in nature and emanate at 45° from the top and bottom corners. These features, which do not appear to correspond to the traces of either the {110} or {112} slip planes, appear early in deformation and persist throughout. A second type of contrast feature lying roughly perpendicular to the above features is observed. This feature, which is characterized by relatively smaller changes in orientation (~0.5°), increases in number density and decreases in spacing with strain. Observed rotations are about the $[1\bar{1}0]$ axis. Of particular interest are the *alternating orientation changes* observed upon crossing several of these features. This suggests the existence of networks of dislocations with net alternating sign that are required to accommodate the observed rotations.

Rotation maps from the transverse section are distinctly different in appearance from those in the longitudinal plane: they are neither sharp nor straight. However, the rotation maps confirm that the rotations observed above were about the $[1\bar{1}0]$ axis. Alternating orientation changes are also observed on this section. Results will be directly compared with crystal rotations predicted using finite element methods and reviewed in light of the LLNL Multiscale Materials Modeling Program.

This work is performed under the auspices of U.S. Department of Energy and Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Session: F2-4 Room: Cascade 123 **Time:** T9:30a-11:30a
Chairs: *J. P. Hirth (WSU) & R. Thomson (NIST)*

A Statistical Approach to the Problem of Deformation in Metals

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National Institute of Standards and Technology, USA

In order to develop a physically based mechanical constitutive law for a deforming metal, one must know how the underlying dislocation structure controls the flow stress. More simply put, how does the stress--strain law reflect the dislocation structure? This is a problem which is not likely to be satisfactorily answered by the extant massive simulations, because it involves the percolation of groups of dislocations (bursts of strain) through a structure composed of a large number of dislocation cells. We address this problem by looking at the deforming solid as a self--organizing critical system, and model the strain as a percolation problem. We will outline the general approach taken and give current results. We will also show how experimental and simulation results will be used as dislocation structure evolution inputs for the modeling.

Dislocation Dynamics In Intermetallics

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Intermetallic alloys display very complex single dislocation processes, many of which are central to the unique deformation characteristics of the material, such as the "anomalous" temperature dependence of the yield strength. Most of these processes are only recently becoming clearly understood. We will discuss two interesting examples, Ni3Al (L1_2) and NiAl (B2).

In Ni3Al, the cross-slip mechanism gives rise to a dynamical phase transition: for small stress, the dislocation becomes completely immobilized by the cross-slip events, while for large stress, cross-slip merely slows the dislocation down. A discrete model has been developed to describe this transition, and mean-field equations derived from it [Chrzan and Daw, Phys. Rev. B, 55, p798 (1997).] Recently, we have obtained an analytic solution to the mean-field equations. The solutions will be compared to existing numerical solutions. The transition is seen to occur for the mean-field solutions, and the exponents and critical-scaling are determined analytically.

In NiAl, experiments [R. Srinivasan et al., Mat. Res. Soc.: High Temperature Ordered Intermetallic

Alloys IV, (v460) p505 (1997)] establish the decomposition of a[111] dislocations as the cause of the loss in yield strength. The decomposition appears to proceed only for particular line directions, and occurs via the nucleation of a small loop on the line, which has a[110] burger's vector on one side and a[001] on the other. Using elasticity theory, we have explored the energetics and dynamics of the decomposition process. We find that a particular path is expected for the decomposition process, which is consistent with the experimentally observed microstructure.

Both cases represent just some of the complex dynamics that dislocations can exhibit in intermetallics.

[*Supported in part by a grant from NSF/Materials Theory.]

Modeling of Dislocations Interacting with a Propagating Crack

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Brown University, USA

Fracture in metals is largely dependent on the plastic zone around a crack tip. Although continuum plasticity theory can give a useful description of a large part of the plastic zone, at sufficiently small distances from the tip, the elastic interaction between the dislocations and the crack control the fracture behavior and the brittle-to-ductile transition. The present study deals with a mesoscopic simulation of the evolution of the plastic zone around a propagating crack tip using discrete dislocations.

The problem we consider is an elastic body under plane strain, which contains dislocations confined to a region close to the crack so that small-scale yielding applies. At the boundary, tractions and/or displacements can be prescribed corresponding to the linear elastic, mode I K-field. All dislocations are assumed to be of edge character, and are treated as line singularities in an elastic material. To model crack growth, a cohesive surface is included ahead of the crack. The traction-separation law used over this surface is motivated by atomic de-bonding. The solution method starts out from analytical stress and strain fields of edge dislocations in a half-space, with the traction-free surface representing the open crack faces. The remote boundary conditions and the conditions ahead of the crack tip are enforced through a complementary finite element solution. The following dislocation properties are incorporated in the model. A linear drag relation is used for the dislocation motion; new dislocation pairs are generated by simulating Frank-Read sources; annihilation of dislocations occur when two opposite dislocations become within a critical distance, and dislocations can get locked at obstacles in the material.

Dislocation Dynamics Simulations in the Presence of Interacting Cracks

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Marmara University, Turkey

Understanding the interaction of different kind of micro-scale imperfections and defects is important in explaining the yielding and failure mechanisms in materials. The failure of a material under any type of loading will initiate from some micro-scale imperfections and develop until the macro-scale observation of failure or deformation is observable. Accurate analysis of the elastic field in a material where multiple of these imperfections are available and interacting may lead to accurate models for failure prevention and the history of plastic zone development. It is known that the presence of multiple cracks is very widely observed in practice and greatly effects the fracture toughness of some materials. Moreover high stress concentration areas such as crack tips are the places where high dislocation mobility can be observed. Therefore crack interaction case is extended one step further to develop a computer simulation technique based on molecular dynamics in the presence of interacting multiple cracks. The effect of interacting multiple finite cracks in an infinite planar domain on the evolution of dislocation structures in the fracture process zone is investigated as functions of magnitudes of applied stresses and lengths, orientations and relative positions of multiple cracks. Dislocation structures, dislocation distribution and strain rates results are presented as functions of applied stresses and crack related parameters. Analyzing the molecular scale edge dislocation movements around the cracks is an important step in explaining the larger scale phenomena such as the shape and development of the plastic zone and crack shielding or propagation.

Moreover by modeling some microcracks by superdislocations in continuum mechanics sense so that numerical complications to be avoided due to too many microcracks in the solution process, and analyzing their effect on the stress intensities at the main crack tips will result simplified analysis at the domains where high concentration micro-cracks observed.

Laser Induced Deformation Patterns in Films and Surfaces

Walgraef, D.J.
Free University of Brussels, Belgium

The coupling between surface deformation and defect motion is at the origin of deformation patterns in thin films and surfaces under laser irradiation. We analyze the dynamics of laser-induced vacancy densities and deformation fields in thin metallic films, and show how it triggers deformational instabilities, in the case of uniform and focused irradiation. Pattern

selection analysis is performed, through linear, nonlinear and numerical methods. In irradiation with extended beams, we show that, according to the relative importance of nonlinearities arising, on the one side, from the defect dynamics, and, on the other side, from the bending dynamics, square, hexagonal or even quasi-periodic patterns are selected. It appears furthermore that one-dimensional gratings are always unstable in isotropic systems. In irradiation with focused laser beams, rose deformation patterns, naturally arise in this model. The petal number in the pattern increases with laser intensity, in qualitative agreement with experimental observations. These results claim for more systematic and quantitative experimental investigations of deformation patterns induced by laser irradiation.

Session: F2-5 Room: Cascade 123 **Time:** T1:00p-3:00p
Chairs: *J. Y. Shu (LLNL) & D. Walgraef (Brussels)*

Gradient Deformation Models at Nano, Micro and Macro Scales

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A review of recent gradient models of material deformation advanced by the author and his co-workers and applied at various levels ranging from nanoscale to macroscale is given. The relevance of some general ideas such as the mixture concept of superimposed states, the selforganization of internal variables and the role of higher order strain or stress gradients is pointed out by means of examples for conventional and novel materials.

The mixture concept of superimposed material states is utilized to model the strength of nanostructured metals and the inverse Hall-Petch behavior. One material state corresponds to the grain interior and the other to the large portion of the grain boundary space surrounding the nanometer size grains. If the assumption is made that each one of these two material states obey Hooke's law of classical elasticity and that they interact mechanically through an internal body force which is proportional to the relative displacement of the two phases, a gradient modification of Hooke's law is obtained and a special theory of gradient elasticity is derived. It is suggested that these models may be used to describe material behavior at the nanoscale.

A complete balance law for the internal variables argument is formulated leading to an evolution equation containing a diffusion-like term which is utilized to interpret deformation patterning at the microscale and the selforganization of dislocations, voids, and other structural defects. An adiabatic elimination argument for the internal variables with diffusive transport is used to produce higher order variables of equivalent plastic strain into the constitutive equation for the macroscopic flow stress. This gradient-dependent expression is utilized to derive various strain gradient models of deformation or flow theories of plasticity. A comparison with other recently published strain gradient plasticity models is made and specific examples of material behavior and configuration are considered.

Strain Gradient Effects in the Deformation of Metal-Matrix Composites

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Barlow, C.Y.
Cambridge University, England

A Joint numerical and experimental investigation is conducted into the deformation of a whisker-reinforced aluminum-based metal-matrix composite. The lattice rotation distribution around the micron-sized whiskers is obtained in thin foils by a TEM technique, using semi-automated analysis of Kikuchi patterns to determine local matrix orientations around whiskers. It is also calculated by the finite element method based on a unit-cell analysis of a metal single crystal containing a rigid whisker. The matrix material is first characterized by the classical scale-independent crystal plasticity theory. It is found that the experimentally measured lattice rotation distribution has a spatial gradient much smaller, by as much as an order of magnitude, than the FEM prediction. An attempt is then made to improve the accuracy of numerical calculations using a strain gradient crystal plasticity theory. The strain gradient theory is based on the notion of elevated hardening due to geometrically necessary dislocations and it accounts for both strain hardening and strain gradient hardening. The crystal theory contains constitutive length scales, typically on the order of microns. The deformation thus predicted exhibits a strong dependence on the size of the whisker in relation to a constitutive length scale. It is found that for a whisker with a diameter close to the length scale, the strain gradient theory is able to predict a spatial gradient of the lattice rotation which is several times smaller than that predicted by the classical theory and agrees much better with the experimental results. On the other hand, when the whisker diameter is much larger than the constitutive length scale, the strain gradient theory predictions approach those of the classical theory. Furthermore the strain gradient theory is able to predict a strong dependence of the yield strength of the composite on the size of the whisker.

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Computational Modeling of Dislocation Based Gradient Plasticity

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In single crystals of ductile materials macroscopic deformation patterns occur which are characterized by localized modes, for example, necking in tension or highly localized shearing in tension or compression. At a microscale localization manifests itself by the occurrence of slip lines induced by dislocations or defects in the crystal lattice. Conventional computational models for the modelling of localized failure processes in crystalline materials lack a characteristic length. In case of multiple slip in a crystal the absence of a characteristic length scale leads to mesh-dependent results, i.e. the orientation and width of slip bands and shear bands are influenced by the discretization process. Furthermore, microstructure development, for example, dislocation cells and microslip bands on the length scale of the mean distance between dislocations, cannot be predicted. In the lecture it will be demonstrated that the introduction of the microstructure into crystalline plasticity models has important advantages in the modelling of localized shearing and dislocation structures. The motion of dislocations is determined by an advection-diffusion-reaction equation, in which transport phenomena, nonlocal dislocation interaction and coupling between micro- and macroscale is incorporated. This so-called dislocation based gradient plasticity model will be used for the analysis of double-conjugated slip.

Multiscale Polycrystal Plasticity

McGinty, R.D. and McDowell, D.L.
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The behavior of polycrystalline metals is manifested across a range of length scales. In the great majority of applications to date, polycrystal models have been built up assuming that the grain is the fundamental unit of deformation, invoking some sort of self-consistent approximation to account for its interaction with neighboring grains among an ensemble to construct local constitutive relations for both stress-strain behavior and evolution of crystallographic texture. More detailed applications have discretized the grain in order to study the role of lattice rotation that arises from crystallographic mismatch. Recent work by Butler and McDowell [1] has addressed the subdivision of the grains by geometrically necessary dislocation boundaries, asserting that they accommodate much of the misfit strain due to local crystallographic misorientations within grains.

To model both texture evolution and stress-strain behavior, the ideal constitutive formulation would start at the level of crystallography (e.g. crystal plasticity), and build up a set of basis functions that are consistent with a physically based averaging process. Although tempting to conclude that an individual grain offers the fundamental length scale to build upon, this is not the case. Due to grain subdivision processes and formation of low (free) energy dislocation substructures, the appropriate reference length scale refines continuously during plastic flow, as do the scales for localized shear deformation. In turn, the contribution of this refinement process to the interaction of misoriented crystallographic regions becomes much more diffused in nature compared to the interactions between distinct grains in the initial stages of plastic deformation in the previously undeformed polycrystal. Accordingly, the collective behavior of a set of initial grains may differ substantially from that assumed in polycrystal plasticity calculations which maintain the original grain boundaries to demarcate jump discontinuities in lattice orientation. Although clusters of 10-20 grains may result in quite inhomogeneous deformation behavior early in a strain history, it is expected that subdivision will lead to increasing homogeneity of hardening and deformation at larger strains. The heterogeneity that affects macroscopic localization behavior then emerges from clusters of grains rather than localization in individual grains. Shifts and distortion of the macroscopic flow potential arise from the action at collective length scales. A variable resolution theory is therefore potentially useful. In this paper, we describe a robust, fully implicit computational implementation of hyperelastic crystal plasticity [2]. An exponential mapping is introduced to enhance accuracy of the slip system rotation associated with the antisymmetric part of the plastic velocity gradient. Concepts of decoupling the scales of flow and hardening are introduced to facilitate computational expediency without loss of accuracy, and to incorporate collective effects that scale with intragranular and intergranular interactions.

[1] Butler, G.C. and McDowell, D.L., "Polycrystal Constraint and Grain Subdivision," Symp. on Failure Mechanisms in Multiphase Materials, ASME Winter Annual Meeting, Atlanta, Nov. 17-22, 1996.

[2] Cuitino, A.M. and Ortiz, M., 1992, "Computational Modeling of Single Crystals," Modelling Simul. Mater. Sci. Eng., Vol. 1, pp. 225-263.

Session: F2-6 **Room:** Cascade 123 **Time:** T3:30p-5:30p
Chairs: *L. J. Sluys (Delft) &*
A. Benzerga (Ecole des Mines de Paris)

Constitutive Modelling of Inelastic Solids for Plastic Flow Processes under Cyclic Dynamic Loadings

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Polish Academy of Sciences, Poland

The main objective of the paper is the description of the behaviour and fatigue damage of inelastic solids in plastic flow processes under dynamic cyclic loadings. Experimental motivations and physical foundations are given. Recent experimental observations for cycle fatigue damage mechanics at high temperature of metals suggest that the intrinsic microdamage process does very much depend on the strain rate effects as well as on the wave shape effects. The microdamage process has been treated as a sequence of nucleation, growth and coalescence of microcracks. The microdamage kinetics interacts with thermal and load changes to make failure of solids a highly rate, temperature and history dependent, nonlinear process.

A general constitutive model of elasto--viscoplastic damaged polycrystalline solids is developed within the thermodynamic framework of the rate type covariance structure with finite set of the internal state variables. A set of the internal state variables is assumed and interpreted such that the theory developed takes account of the effects as follows: (i) plastic non--normality; (ii) plastic strain induced anisotropy (kinematic hardening); (iii) plastic spin; (iv) softening generated by microdamage mechanisms; (v) thermomechanical coupling (thermal plastic softening and thermal expansion); (vi) rate sensitivity.

To describe suitably the time and temperature dependent effects observed experimentally and the accumulation of the plastic deformation and damage during dynamic cyclic loading process the kinetics of microdamage and the kinematic hardening law have been modified. The relaxation time is used as a regularization parameter. By assuming that the relaxation time tends to zero, the rate independent elastic--plastic response is obtained. The viscoplastic regularization procedure assures the stable integration algorithm by using the finite difference method. Particular attention is focused on the well--posedness of the evolution problem (the initial--boundary value problem) as well as on its numerical solutions. Convergence, consistency, and stability of the discretised problem are discussed. The Lax--Richtmyer equivalence theorem is formulated and conditions under which this theory is valid are examined. Utilizing the finite difference method for regularized elasto--viscoplastic model, the numerical investigation of the three--dimensional dynamic adiabatic deformation in a particular body under cyclic loading condition is presented. Particular example has been considered, namely a dynamic, adiabatic, cyclic loading process for a thin steel plate with small rectangular hole located in the centre. Small two regions which undergo significant deformations and temperature rise have been determined. Their evolution until occurrence of final fatigue fracture has been simulated. The accumulation of damage and equivalent plastic deformation on each considered cycle has been obtained. It has been found that this accumulation distinctly depends on the wave shape of the assumed loading cycle.

Coalescence-Controlled Anisotropic Ductile Fracture

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Hot--rolled steels often exhibit anisotropic behavior of both plastic flow and damage evolution. They may contain large manganese sulfide inclusions elongated in the primary working direction thus leading to values of ductility and fracture toughness in transverse T (width) direction significantly lower than in longitudinal L (rolling) direction. Experiments were carried out to evidence such a difference. Mechanical tests were performed on smooth and notched tensile bars and compression cylinders. L, T and LT (i.e. at 45^0 to the rolling axis) directions were tested. CT specimens were used to characterize crack initiation and propagation in both configurations L-T and T-L. Inter—inclusion mean spacings were characterized by quantitative metallography along the different directions.

Classical modelling of ductile fracture uses void growth models with failure criteria based on a critical void growth ratio. These approaches implicitly assume that voids still grow until ``slipping--off''. Experimental investigations on void coalescence 1 showed that at least two microscopic mechanisms, void impingement or void--sheet process, could lead to the final stage of dimpled fracture. The occurrence of either of them could have a strong influence on material toughness regardless to the other. In particular, the void sheet mechanism is well known to be extremely deleterious. The mean spacing between inclusions, combined to the matrix--inclusion interface strength, has been shown to be a selective parameter of coalescence process. On the other hand, inclusion spacing has been shown to strongly influence toughness of metals 1 for a given volume fraction of inclusions.

Void coalescence by void--sheet mechanism has been analyzed in 2. The analytical approach is based on strain localization in a porous ductile medium (such as Gurson's) as pioneered by Rudnicki and Rice. Thomason 3 used an approach where coalescence is the

result of necking down the intervoid matrix. This is accounted for by introducing a second strong dilational--plastic response plus the weak one due to dilute porosity, in a plastic limit--load failure model. A critical porosity is derived from both models as being a function of stress triaxiality.

The aim of this paper is first to emphasize the void--coalescence contribution in the damage behavior of metals. It is also to compare both proposed models and to check their ability to incorporate the void spacing in order to explain the anisotropic fracture at a macroscopic scale. For this purpose, finite element (FE) calculations were performed to model the behavior of smooth, notched and cracked specimens. The constitutive equations are based on a Gurson—like model which incorporate plastic anisotropy 4. Critical void volume fraction for the onset of coalescence was evaluated based on the previous models as a function of stress triaxiality ratio and the mean particles

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2. Leblond, J. and Perrin, G., (1991), In *Plasticity 3rd symposium*, 233--236.
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Yield Strength Asymmetry Predicted Using Polycrystal Elastoplasticity

Barton, N., Dawson, P. and Miller, M.P.
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Since the 1960's, it has been known that elastoplastic polycrystal models exhibit asymmetries in the yield strength for polycrystals that have been prestrained. The stress responses in tension and compression after preloading in tension show Bauchinger-like behavior in that the compressive response exhibits yielding at a lower stress level than the tensile response upon reloading. Further, the knee of the reloading stress-strain curve is more gradual for compression than for tension. The origins of this response reside in the assumption that links the macroscopic deformation to the deformations in individual crystals. More precisely, the residual stress field induced with plastic straining by the presence of softer or harder crystal orientations biases the response on reloading. While the earlier work pointed to the polycrystalline origins of the asymmetry, it left unanswered the assessment of its sensitivity to the particular linking assumption used in the modeling. However, due to the strong influence of the linking assumption on the crystal stresses, the sensitivity is expected to be appreciable. In this paper we present the results of an examination of the influence of the linking assumption on the magnitude of the computed yield strength asymmetry of prestrained polycrystals. Simulations based on upper (Taylor) and lower (equilibrium-based) bound linking assumptions are compared to elastoplastic finite element computations in which elements constitute individual crystals. The finite element model maintains compatibility while satisfying equilibrium in a weak sense. The influence of neighboring crystals is explicitly treated in the finite element simulations. The strength of the predicted Bauchinger effect does depend on the linking assumption, with 'compatibility first' models showing more significant yield strength asymmetries.

Microscopic Expressions of Balance Equations for Macroscopic Continuum Based on Lattice Dynamics

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Recently, the studies to grasp the macroscopic behavior of materials from the microscopic viewpoint of atomic level have been actively done by many researchers. Though the method to connect the microscopic quantities to the macroscopic balance equations and the macroscopic quantities used in solid mechanics is always necessary in such approaches, a desirable method has never been developed theoretically. In this study, a meso-mechanics is proposed to obtain the microscopic expressions of macroscopic balance equations and quantities for solids on the basis of lattice dynamics. The macroscopic body of a solid is modeled as an assembly of atoms in which the force acting on an atom is given by the interatomic potential. A mesodomain which contains a great number of atoms is introduced into the macroscopic body so that kinematical and mechanical quantities of an atom can be averaged in this domain. By attaching the averaged values to the mesodomain and regarding it as a material point macroscopically, the body of solid results in a continuum. Macroscopic mechanical balance equations and natural boundary conditions for not only stress but also higher-order stresses are derived by using the principle of virtual power described with the averaged values. The stress and higher-order stresses can be expressed with the microscopic quantities of atoms comparing the equations and conditions mentioned above with the conventional ones.

Furthermore, the conservation law of energy is formulated with microscopic quantities for a mesodomain in which the velocity of an atom is dividing into the macroscopic motion and thermal one. Then the microscopic expression of heat flux is also obtained from the energy equation. By taking notice of the relationship between the microscopic expressions of heat flux and the higher-order stress power, it is clarified that the heat flux is equivalent to the sum of higher-order stress powers. In other words, when the microscopic force acts on the mesodomain, the power due to the averaged value of the force is the usual macroscopic stress power and the power due to the

fluctuation of the force is the heat flux. If the higher-order stress power of the first order is separated from the heat flux in the energy equation, it becomes the energy equation of Cosserat continuum. Additionally, the expressions of internal energy, stress, higher-order stresses and heat flux are useful in obtaining macroscopic quantities from numerical solutions calculated by the molecular dynamics.

The results obtained here are summarized as follows.

1. The macroscopic balance equations expressed with microscopic quantities are derived by dividing the kinematical quantity of an atom into the macroscopic motion and thermal one.
2. The heat flux is equivalent to the sum of higher-order stress powers. The value of heat flux for the material of grade n decreases in comparison with one of the simple body, when the higher-order stress powers over the nth order are separated from the conventional heat flux.

A Thermodynamical Theory of Plastic Spin and Internal Stress with Dislocation Density Tensor

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Washington State University, USA

The plastic spin has recently attracted considerable attention as a proper spin of the corotational constitutive equation of elastoplasticity for kinematic hardening model with internal stress. However, the plastic spin and internal stress have never been investigated thermodynamically because of no quantities conjugate to them. The issue may arise from the lack of discussions on the fact that these internal variables have a common origin in the dislocation motion.

In this study, a thermodynamical theory of plastic spin and internal stress at finite strain is developed by introducing the concept of dislocation density tensor. The thermodynamically appropriate intermediate configuration for plastic spin is strictly presented as a configuration pulled back from the current one by rigid and elastic rotations. In this configuration, the thermodynamical rates such as the deformation rate and dislocation drift rate can be decomposed into the rates of a strain measure for elasticity which is a reversible thermodynamic state variable and deformation measures for plasticity which are irreversible quantities dependent on the stress path. By selecting newly the dislocation density tensor as an argument of free energy, the thermodynamical forces such as stress, effective stress with back stress and microstress caused by the dislocation structure are defined and then the balance equations for these forces are obtained by use of the principle of virtual power. The thermodynamically consistent constitutive equations for elastic strain, plastic stretching and dislocation drift rate are rigorously derived on the basis of two fundamental principles of thermodynamics, the principles of increase of entropy and the maximal entropy production rate. Moreover, it is shown that a characteristic length scale associated with the equivalent dislocation density influences to the work hardening in the present theory.

The results obtained here are summarized as follows.

(1) The balance equation of microstress and the constitutive equation of dislocation drift rate are newly added to the conventional basic equations system of elastoplasticity with effect of kinematic hardening. The former contributes to the determination of back stress and the latter assumes the role of the constitutive equation for plastic spin.

(2) The present self-consistent theory includes a length scale expressing size effects due to the equivalent dislocation density although the stress tensor is symmetric.

Symposium F3
Superplasticity and Superplastic Forming: Characterization, Modeling and Applications
Organizers
M. Khaleel, M.T. Smith
Pacific Northwest National Laboratory, USA
&
C.H. Hamilton
Washington State University, USA

Session: F3-1 Room: CUB 224 **Time:** M4:00p-6:00p
Chairs: *T. R. McNelley (Naval Postgraduate School) & T. Bieler (Mich. State U.)*

Initiation And Early Stages Of Cavity Growth During Superplastic And Hot Deformation

Ghosh, A.K. and Bae, D-H.
The University of Michigan, USA, and
Semiatin, S.L.
Air Force Research Laboratory, USA

The formation and growth of internal voids in metallic alloys are of considerable concern in components produced by superplastic forming and hot forming processes. Grain boundary cavitation, generally observed under conditions in which grain boundaries are weaker than grain interior, results from strain concentrations around non-deformable particles and/or misoriented hard second phase located at grain or colony boundaries. Careful examination of microstructures of aluminum and titanium alloys show that most voids are "nucleated" due to incompatible deformation between phases, although a few cavities do preexist in certain alloys. High levels of local hydrostatic tension in regions of incompatibility lead to rapid dilatational growth initially, followed by a slower growth rate due to reduced plastic constraints as voids expand. This initial growth kinetics applies suitably over a wide range of temperatures, particularly where diffusional growth mechanisms are not appropriate. Detailed experimental studies, utilizing image analysis of incrementally tested specimens as a function of test temperature and strain rate, have revealed how the population of cavity nuclei increase with increasing strain rate and decreasing temperature, and how this, in turn, modifies the growth rate of individual cavities. New simplified models of growth of individual cavities are in good agreement with the evolutionary details of cavity size distribution, and thus provide an insight into observed variations in the overall cavity volume vs. strain under various test conditions. This work provides a basis for predicting the evolution of void size and overall void volume under a variety of forming conditions. (Work performed under support from US Dept of Energy grant FG02-96ER45608-A000, and US Air Force Contract F33615-94-C-5804 for sabbatical leave appointment of A.K. Ghosh at AFRL).

Characterization of Grain Boundary Evolution During Processing and Deformation of Superplastic Aluminum Alloys

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One of two distinct microstructural transformation processes may enable superplastic response in an aluminum alloy, depending upon its composition and thermomechanical history. The transformation behavior in alloys that respond in the same manner as Supral 2004 has been termed #continuous recrystallization#. High-angle grain boundaries develop as interfaces between symmetric variants of texture components when grains subdivide during large-strain deformation. Low- and moderately-misoriented boundaries develop by dislocation reactions, resulting in bimodal grain boundary misorientation distributions. Changes take place gradually and homogeneously throughout the deformation microstructure during annealing. During elevated temperature deformation, the stability of texture components near the Brass orientation suggests that slip and grain boundary sliding processes contribute in varying proportions, depending on temperature and strain rate. Alternatively, aluminum alloys such as 5083 and 7475 transform via recrystallization processes involving the heterogeneous formation and subsequent growth of grains by the migration of high-angle grain boundaries from the deformation zones surrounding coarse precipitate particles. The stable end orientations in the texture developed during deformation processing are replaced by weak recrystallization components. Corresponding grain boundary misorientations tend to be random. Changes in texture during elevated temperature deformation can also be described in terms of contributions from slip and grain boundary sliding. The development of thermomechanical processing methods for superplastic aluminum will be reviewed in light of recent advances in understanding of the phenomena involved in recrystallization.

A Mechanism for Deformation-Enhanced Grain Growth During Superplastic Deformation

Hamilton, C.H.
Washington State University, USA

It is well documented that grain growth rate during high temperature exposure is dramatically increased by the imposition of superplastic deformation, a characteristic which has been termed "dynamic grain growth" (DGG) or "deformation-enhanced grain growth" (DEGG). That latter term will be used here.

For superplastic materials, DEGG occurs is much faster than for the "static grain growth" (SGG) and usually dominates the grain size changes observed in superplastic deformation (SPD). This microstructural evolution has been shown to be important in SPD since the flow stress is a strong function of grain size, and DEGG leads to strain hardening and affects the necking and localization in SPD. There have been a number of mechanisms proposed to explain DEGG, but there they are not entirely satisfactory, and the mechanism remains in question. In this study, a suggested mechanism of altered boundary driving force resulting from grain elongation is studied through a numerical solution to the problem. A two-dimensional model is developed which expresses the boundary energy driving forces as forces acting at the grain triple junctions, and a numerical solution focuses on the behavior of a grain with various numbers of sides and connected at the nodes to surrounding grains. The model produces grain boundary migration and grain size changes that are consistent with SGG and DEGG . Model calculations show that grain elongation alters the driving forces acting on the grain boundaries, and cause grains with fewer than 6 sides to shrink faster and those with more than 6 sides to grow faster when compared to SGG.

Role of Local Composition on Interfacial Sliding

Vetrano, J.S., Henager, Jr., C.H. and Bruemmer, S.M.
Pacific Northwest National Laboratory, USA

The processes of grain boundary sliding has been shown to depend on the composition of in the boundary plane and the near-boundary region. Tensile testing of Al-Mg alloys with and without the presence of Sn on the grain boundaries has shown that the presence of Sn increases the propensity of the boundaries to slide. The process of grain boundary sliding itself has also been shown to re-distribute solute atoms in a heterogeneous fashion along internal interfaces and triple points. Interactions between sliding boundaries and solute atoms is thought to be caused by localized diffusion processes. Implications of these interactions on alloy design and post-formed properties will be discussed.

The Effect of Threshold Stresses on High Strain Rate Superplastic Formability when Thermal and Strain Rate Gradients Exist

Bieler, T.R.
Michigan State University, East Lansing, USA

Temperature dependent threshold stresses that define the low end of region II is a significant feature in materials that exhibit high strain rate forming capability. In low strain-rate superplastic materials, superplastic behavior is sometimes a result of a transition between well-defined deformation mechanisms in regions I and III. In contrast, high strain-rate superplastic materials frequently have well-defined superplastic mechanisms in region II, and region I represents a transition between the superplastic mechanism and a region 0 creep mechanism that is frequently not even observed due to a lack of low strain rate data. In these conditions, the transition between region II and region I can be quite sharp, leading to a rapid drop in strain rate if the stress is not maintained at a high enough level. In order to properly predict material flow behavior in these technologically important low strain-rate conditions, constitutive models must represent this threshold stress phenomena accurately. In superplastic forming of complex shapes, thermal and strain rate gradients will lead to portions of the material deforming in or near region I conditions, where the ductility is much lower. Although these conditions may not lead to failure of the material during forming, the differences in flow behavior can lead to cavitation damage that could influence post forming reliability of the part. In this context, a criteria for cavitation is valuable for predictive modeling. Data will be presented that illustrate how threshold stress and cavitation criteria can be defined in a form useful for constitutive models.

Session: F3-2 Room: CUB 224 **Time:** T9:30a-11:30a
Chairs: *D. G. Sanders (Boeing) & W.C. Simmons (Army Research Office)*

Aerospace Manufacturing Challenges For Superplastic Forming In The Twenty-First Century

Sanders, D.G.
The Boeing Company, USA

Superplastic Forming (SPF) of titanium alloys, especially type AB-1 (6 Al – 4 V), has become a highly leveraged process for the aerospace industry. The Boeing Company has developed this manufacturing and design technology to replace conventional built-up assemblies with SPF monolithic structure. This has resulted in cost, weight and performance gains on all of Boeing's commercial jetliner products. Many successes have been made. However, the opportunity for improvement has become a recurring discussion topic due to the developmental nature of the process and the lack of certain supporting technologies. SPF is still relatively in its infancy and many opportunities for improvement have been identified.

The academic community has approached SPF research with wide ranging materials development programs. A host of new Superplastic aluminum, titanium, metal matrix composite, powder metal alloys, intermetallics, fiber reinforced alloys and ceramic material systems have been investigated. These programs have been aimed primarily at high technology industries of the future and aerospace applications such as the National Aerospace Plane.

Very little research is being performed on current SPF manufacturing fundamentals. In general, SPF industrial manufacturing technology has lagged behind the development of these advanced SPF materials and novel design concepts. This has led to the current situation, in which the factories that must produce SPF components are struggling to overcome a host of challenges.

As we move towards the twenty-first century, the focus of SPF technology innovation is shifting. Commercial SPF research and development activities are moving away from the traditional objectives of advancing new materials and structural design development. This paper has been written to identify the many new categories of research that will be explored in coming years. These areas include the following:

- Development of High Temperature Oxide resistant and creep resistant CRES alloys for use in cast/machined dies
- Fast die change methods, setup reduction
- Inexpensive SPF press design and control system improvements
- Cast ceramic tooling (fused silica and other materials)
- Titanium sheet cost reduction (at the mills)
- Finite Element Modeling techniques

Review Of Army Interests In Superplasticity

Simmons, W.C.
Army Research Office, USA

Highlights of the Army Research Office program in superplasticity theory, practice and applications will be reviewed. Superplastic effects in metals, intermetallics, ceramics and composites are of interest to the fabrication of components and to materials response at high strain rates. Lightweight, near-net-shape and economical processing routes are desirable.

Research Toward the Increased Use of Superplastic Forming in Lightweight Structures

Smith, M.T.
Pacific Northwest National Laboratory, USA

Considerable research has been performed in recent years to enhance material models and finite element codes to accurately simulate the superplastic forming (SPF) of sheet metal components. Accurate simulation of SPF will help to reduce or eliminate the costly (and time-consuming) trial and error process that has often been used to development tooling and forming cycles for SPF. Efficient modeling and simulation capabilities will allow industry to design components with significantly reduced part count, lower material usage, and improved performance characteristics.

This paper summarizes research performed at the Pacific Northwest National Laboratory (PNNL) to integrate SPF model development with research in improved aluminum alloys for SPF. The goal of this work has been to increase the use of aluminum alloys in lighter-weight transportation structures. The objectives of PNNL's research have been: 1) to develop and characterize competitively priced aluminum alloys for SPF applications in industry, 2) to improve numerical models to accurately predict the optimum forming cycle for reduced forming time and improved part quality, and 3) to verify alloy performance and model accuracy with forming tests conducted in PNNL's Superplastic Forming User Facility. This paper summarizes the progress made toward these objectives and assesses the direction of continued SPF development needs.

Integrated Design Environment for the Manufacture of SPF Components

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Florida A&M - Florida State, USA

Superplastic Forming (SPF) is an extremely powerful manufacturing method for forming near-net complex shapes with less number of joints, and produces structurally stable and light weight components. Presently, the potential of SPF is not fully realized, and is resorted to only when all other conventional manufacturing methods fail to meet the design need. There are a number of non-aerospace applications where SPF offers potential alternative to other forming methods. Those applications have come about more by accident than by choice. In this work, a computer integrated design and manufacturing environment is proposed so that SPF can be considered as a viable processing method at the design stage. Integration of design (Pro-E) with forming and stress analysis (MARC) with material modules (MATDATA) is demonstrated through practical examples. A web browser based interface that integrates the various tools in SPF is also presented.

SPF Application Challenges and Opportunities - A Part Manufacturer Prospective

Kistner, M.
GKN Westland, USA

Session: F3-3 Room: CUB 224 **Time:** T1:00p-3:00p
Chairs: *J. Will (Boeing Company) &*
M. K. Khraisheh (King Fahd U.)

Advanced Multi-Sheet SPF/DB Fabrication

Will, J.
The Boeing Company, USA

Single sheet, superplastically-formed components have been utilized in structural applications for some time while multi-sheet structures have not. Part of the reason is the scarcity of data describing mechanical behavior of multisheet structural elements. In this paper, we describe the design, fabrication and mechanical properties of two four-sheet titanium alloy panels produced by laser welding/superplastic forming/diffusion bonding (LW/SPF/DB). The panels were constructed of Ti-62222S face sheets with Ti-64 core sheets in a sine-wave geometry. Testing consisted of face sheet tension, panel edgewise compression, and panel fatigue. The mechanical properties, microstructures and failure modes of the panels were characterized.

Bulge Forming of Superplastic Sheet Materials Under Strain Rate-Controlled Pressure Profiles

Khraisheh, M.K.
King Fahd University of Petroleum and Minerals, Saudi Arabia

There has been an increasing interest in superplastic forming in recent years as it becomes a viable manufacturing process with vast applications in the aerospace and the auto industries. Bulge forming is the most common technique used in forming superplastic sheet materials, where a pressurized gas is used to form the sheet material to the desired shape. Most of the work that has been done to analyze this process considered constant forming pressure, and little effort has been made to develop optimum variable pressure forming profiles. In this study, the bulge forming performance of Pb-Sn superplastic sheet materials is evaluated under different forming pressure profiles. In addition, an optimum pressure profile based on variable strain rates is proposed. Results of forming time, achieved amount of deformation, and thinning behaviour are reported for the different forming pressure profiles. Not only the forming time was significantly reduced, when forming with the optimum pressure profile, but the integrity of the formed part was also maintained. Furthermore, the results clearly show that uniaxial models cannot successfully predict the actual forming behaviour. In fact, the one dimensional strain rate hardening relation along with von Mises criterion predicts failure at a much higher time than the actual case.

Retention Of Texture In Superplastic Forming Of A Hemisphere From Commercial Ti-6Al-V Plate

Sundaresan, R., Krishnaswamy, W., Singh, A.K. and Rao, K.M.
Defence Metallurgical Research Laboratory, India

Titanium alloy Ti-6Al-4V in commercial mill product form often exhibits superplasticity. Plates of 6 mm thickness were evaluated for superplasticity by extensive evaluation of the microstructure and the strain rate sensitivity index m. The plates were superplastic formed to different extents of a hemispherical shape. The components were evaluated for the phase distribution by microstructure analysis and x-ray diffraction. Based on the indication of texture from XRD, detailed texture analysis was done by pole figure and orientation distribution function plots. It is seen that the texture can be gainfully used to enhance the mechanical strength of spherical bottles made by SPF.

Superplastic Forming Of Titanium 6Al-2Sn-2Zr-2Mo-2Cr-.2Si

Gillespie, F.S.
The Boeing Company, USA

Titanium 6Al - 2Sn - 2Zr - 2Mo - 2Cr - .2Si (Ti 6-"Quad"2) is one of three titanium alloys that are showing considerable promise as structural Superplastic materials. Ti 4.5Al - 3V - 2Fe - 2Mo (SP700), Ti 4Al - 4Mo - 2Sn - 0.5Si (IMI 550) and Ti 6Q2 show potential advantages in reducing forming temperatures, reducing forming time, and increasing tensile properties compared to Ti 6Al - 4V. A constant strain rate cone die is used to investigate the superplastic properties of Titanium 6Q2 and compare them to those of Titanium 6Al - 4V. Strains and strain rates are measured at temperatures of 1450 F (790 C), 1550 F (840 C), and 1650 F (900 C). Tensile properties following selected age temperatures are reported. It is recommended that efforts continue toward using SPF Ti 6Q2 for flight hardware.

Diffusion Bonding of Superplastic Materials: Theory and Practice

Pilling, J., Ridley, N. and Wang, J.
Michigan Technological University, USA

Diffusion Bonding prior to superplastic forming allows the fabrication of shell structures with integral internal stiffening structures and gives rise to a lightweight and stiff components. The practice of Db/SPF has been successfully applied to the manufacture of aerospace and other parts in titanium-base, stainless steel and nickel-base alloys. While high strength bonds have been developed in superplastic aluminum-based alloys, the reproducibility of the bond

strength has been woefully inadequate for use in structural applications. Development of the DB pressure/temperature/time cycle has often been carried out using trial and error based on past experience. In this paper we review the various theoretical approaches that have been adopted to calculate the time required to remove interfacial porosity and examine the sensitivity of their predictions to (a) materials properties and (b) surface geometry, as well as compare the predicted bonding cycles with those determined by experiment. We shall demonstrate that the definition of the scale of the initial surface roughness is by far the most important step in accurately predicting bonding times and in developing bonding pressure/temperature/time cycles that preserve a microstructure capable of undergoing post bonding superplastic forming. Experimental findings relating to the effect of geometry, sheet thickness and other process variables will by discussed in relation to superplastic titanium alloys, intermetallics, duplex stainless steels and aluminum alloys.

Session: F3-4 Room: CUB 224 **Time:** T3:30p-5:30p
Chairs: *D. Lesuer (LLNL) &*
M. Jimenez-Melendo (Universidad de Sevilla)

Superplasticity In Nanometals, Nanointermetallics And Nanoceramics: Some Results And Reflections

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University of California, Davis, USA

Fine, equiaxed grain size has been one of the primary prerequisites for superplasticity. Reduction of this grain size has spurred recent investigations on low temperature superplasticity as well as high strain rate superplasticity. Nanocrystalline material provides the ultimate limit to these reduced grain size considerations.

Nanometal, nanointermetallic and nanoceramics were investigated. These materials were produced primarily by ball-milling and subsequent consolidation by severe plastic deformation or by high pressure sintering. Polymer precursor derived amorphous ceramic powders were also consolidated using high pressure sintering.

The mechanical properties were determined either by constant strain rate compression testing in MTS equipment or by tensile testing in a specially designed mini tensile tester with very good resolution for load and displacement. This computer-interface equipment can be used at constant tensile strain rate. The entire tensile specimens were less than 8 mm in length. Preliminary mechanical and microstructural results from this ongoing program will be discussed in the context of the appropriateness of applying the currently available models for superplasticity.

This investigation was supported by NSF-DMR-9630881 and NSF-CMS-96-34179.

Superplastic Behavior Of Yttria-Stabilized Zirconia Ceramics

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The possibility of achieving superplastic ceramics for use in industrial forming applications have attracted considerable interest in yttria- stabilized zirconia polycrystals (YSZP) —as well as in a wide range of ceramics and ceramics composites— in the last few years. Despite the numerous studies on deformation in YSZP ceramics, different, and often conflicting, deformation parameters have been reported in the literature for nominally similar materials. A detailed analysis of available data in fine-grained (grain size $d < 1\ \mu m$) YSZP shows the following points: (i) The low purity materials (residual impurity content above 0.1 wt%) exhibit an apparent stress exponent $n = 2$ over the entire stress range, while the more pure materials display a transition in n from 2 to higher values, and then towards 1, as the stress decreases. This behavior is similar to that found in superplastic metals (regions II, I and 0, respectively). (ii) Unreasonable values of the stress exponent n (up to 5), the activation energy Q (up to 700 kJ/mol) and the grain size exponent (even 0) are found in region I. And (iii) the transition stress between region II and region I decreases when increasing the temperature and/or the grain size.

The values of the creep parameters in region I are hardly compatible with any existing model of high temperature creep. However, they can be reduced to the values found in region II by incorporating a threshold stress into the analysis below which grain boundary sliding does not contribute to strain. A threshold stress formalism is widely used to explain the conventional and the high strain rate superplasticity of metallic alloys. The results of the present investigation imply that the same mechanism controls the deformation process in region I and II; the apparent differences in behavior between the two regions arise from the increasing significance of the threshold stress at low stresses. The threshold stress is tentatively related with yttrium segregation at grain boundaries and its interaction with grain boundary dislocations. In addition, it is shown that the constitutive equation for superplastic flow of YSZP ceramics is identical to that found for metallic systems when lattice diffusion is the rate controlling mechanism, despite the differences between both kinds of materials.

Superplasticity in Laminated Metal Composites

Lesuer, D., Syn, C. and Sherby, O.
Lawrence Livermore National Laboratory, USA

Several studies have shown the possibility of achieving superplastic behavior in laminated metal composites consisting of alternating layers of superplastic and non-superplastic materials. Achieving high rate sensitivity in such a laminate requires the appropriate choice of component materials and component volume fraction as well as deformation under appropriate conditions of strain rate and temperature. In this paper, the mechanics of superplastic deformation in layered materials is examined. The strength of the laminate can be predicted from the law of averages and calculations using such an approach can correctly predict the strain rate sensitivity of the laminate as well as the activation energy. High elongations require achieving high strain rate sensitivity as well as avoiding brittle fracture in the less ductile layer. Various deformation modes will be analyzed including laminates undergoing tension parallel to the layers and compression perpendicular to the layers as well as the response of materials undergoing co-extrusion. Experimental data will be presented and analyzed for superplastic ultrahigh carbon steel (UHCS) laminated with various metals including mild steel, iron, stainless steel, brass and an aluminum bronze.

Cavitation and Fracture Characteristics of Si_3N_4p /Al Alloy Composites Exhibiting High-strain-rate Superplasticity

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Mabuchi, M.
National Industrial Research Institute of Nagoya, Nagoya, and
Higashi, K.
Osaka Prefecture University, Japan

High-strain-rate superplasticity is very attractive for commercial applications because one of current drawbacks in superplastic forming technology is a slow forming rate which is typically ~10^{-4} s^{-1}. Though the origin of high-strain-rate superplasticity is now under hot discussion, it is accepted that high-strain-rate superplasticity is associated with a very small grain size. However, the deformation mechanisms in high-strain-rate superplastic materials appear to be different from those in conventional superplastic materials. A new accommodation process for high-strain-rate superplastic flow is required to continue superplastic flow when the stress concentration is insufficiently relaxed by diffusional flow and/or diffusion-controlled dislocation movement under the given deformation conditions. A liquid phase plays an important role as an accommodation helper in the accommodation mechanisms of high-strain-rate superplasticity, that is, in an assistance to relax stress concentrations caused by sliding. Cavitation and fracture behavior at various conditions for liquid phases are investigated by a quantitative analysis for a high strain rate superplastic materials. It is suggested from an theoretical analysis that diffusion-controlled cavity growth is limited and the plasticity controlled cavity growth is dominant when stress concentrations at triple junctions of boundaries and around reinforcements are relaxed by the presence of a liquid phase, so the cavity growth is significantly slow in a small cavity size range, This view was in agreement with the experimental data of the cavity growth rates.

Effect of Dopants and Impurities on the High Temperature Mechanical Characteristics of Superplastic Yttria-Stabilized Tetragonal Zirconia

Owen, D.
California Institute of Technology, USA

From the earliest reports of superplasticity in yttria-stabilized tetragonal zirconia (YTZ), there have been discrepancies in the reported regarding the characteristics of high temperature deformation. Typically the creep rate is expressed as a function of stress raised to a power 'n,' inverse grain size raised to a power 'p' with an Arrenhius temperature dependence characterized by an activation energy, Q. In these early studies, materials of nominally similar composition and grain size were reported to have different values of n, p and Q. Closer examination of the levels of trace impurities cited revealed that the behavior observed in a given study could be associated with either 'large' or 'small' concentrations of these impurities. Subsequently, more detailed studies of the high temperature creep behavior have resulted in a more complete constitutive description. However, inspite the recognition of the importance of impurities in the high temperature characteristics of YTZ, there is still a lack of fundamental understanding of the effect impurities have on the deformation mechanism. This paper provides a critical assessment of the role of impurities and dopants in the high temperature creep behavior of YTZ. In particular, the role of the impurities play in the observed deformation mechanism, evidenced by the values of n, p, and Q and the deformation rate will be addressed. Experimental observations of a variety of high temperature processes will be used to develop a unified view of these complex high temperature phenomena.

Session: F3-5 Room: CUB 224 **Time:** W9:30a-11:30a
Chairs: *T. Zacharia (ORNL) & R. Sadeghi (MARC)*

Finite Element Modeling Of Superplastic Forming

Sadeghi, R. and Pursell, Z.
San Diego State University, USA

Finite Element modeling of superplastic forming with complex die shapes is developed using analysis procedures of the MARC-MENTAT system, developed by MARC Analysis Research Corporation. The analysis of superplastic metal forming operations requires a model for large deformations of a strongly nonlinear material. Successful computer modeling is shown to accurately predict both material behavior and thinning characteristics of the finished workpiece.

The finite element analysis utilizes a Rigid Plastic Flow formulation in which the effects of elasticity are neglected. A material model based on an empirical relation between flow stress, strain-rate and grain size is incorporated into the analysis [1]. The mechanics of grain growth, which has been shown to be a function of material strain-rate is modeled as well. The effects of grain growth during superplastic deformation are shown to improve the thinning prediction and forming time.

Contact between the die and workpiece is modeled using an improved contact algorithm. The algorithm has been developed for constraining nodes onto a rigid contact surface, which is represented analytically using nonuniform rational B-spline surfaces (NURBS). The use of NURBS has the advantage of continuity of the normal vector along the defined surface and the flexibility to model multiple complex surfaces with a single mathematical description. The use of NURBS eliminates inaccuracies due to discretization, resulting in the reduction in the number of iterations required for solution. The accuracy of the solution is improved while reducing computational time by a factor of two.

The adaptive meshing generation capability within MARC is utilized to further improve the accuracy of the solution. With the use of adaptive meshing, the element is subdivided when one of its nodes is associated with a new contact condition. Once an element is subdivided, internal node degrees of freedom are tied to insure compatibility. After a new mesh is created, the new nodes are checked to determine if they are in contact as well.

[1] Hamilton, C.H., "5083 Al Alloy Constitutive Parameters for Superplastic Deformation." Department of Mechanical and Materials Engineering, Washington State University, rev. 1, Aug. 1993.

Numerical Simulation Requirements for SPF of an Industrial Titanium Part the FIRST TIME EVERY TIME

Bennett, J., Haberman, K. and Piltch, M.
Los Alamos National Laboratory, USA

Modeling of Superplastic Forming

Zacharia, T. and Sarma, G.*
Oak Ridge National Laboratory, USA

Superplastic forming provides numerous advantages in production applications including savings as high as 48 percent above the cost of conventional forming techniques and the attainment of near net shape configurations leading to a reduced amount of scrap. Accurate modeling of deformation processing in the superplastic regime can lead to a better exploitation of these advantages. Enhanced numerical simulation of materials deformation during superplastic forming (SPF) of lightweight materials is an important element in achieving forming rate and cost goals for high production applications. The goal of three times the fuel economy as outlined in the PNGV program will require considerable reduction in the weight of current automobiles. The reduction of vehicle weight to improve fuel economy can be accomplished by developing alternative materials and processes. One potential technology is superplastic forming since it is estimated that the number of components that will go into the making of a car door, for example, can be significantly reduced by about 90 percent with a feasible weight reduction of 50 percent. Mathematical modeling of the superplastic forming process is used to predict the pressurization rate which will result in optimum superplastic formability and to predict the distribution of thickness in the formed part so that producibility can be assessed. Modeling also yields an estimate of forming time, which is needed to estimate the cost of operation. Results of a modeling study at ORNL will be presented. Comparisons of the predictions with experimental observations will also be presented.

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Control of Superplastic Forming Simulations in a Parallel Processing Environment

Johnson, K.I. and Khaleel, M.A. and Smith, M.T.
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van der Walt, P.
MARC Analysis Research Corporation, USA

Finite element simulation has often been used to predict optimum pressure cycles and the final thickness distribution in sheet metal parts formed using the superplastic blow forming process. Typical control algorithms scan the model after each solution increment and adjust the applied pressure to maintain the maximum equivalent strain rate within a specified range. However, these control methods must be modified in a parallel processing environment when the domain decomposition method is used to partition the numerical solution algorithm for multiple processors. This paper presents an overview of the domain decomposition method as implemented in the MARC finite element code. The paper then describes the solution control methods that have been developed for use with the domain decomposition method. Results are presented comparing forming pressure cycles based on several control methods.

Parametric Pressure Profiles for Superplastic Sheet Metal Forming

Lamendola, J.A.
Washington State University, USA, and
Johnson, K.I. and Khaleel, M.A.
Pacific Northwest National Laboratory, USA

The paper describes parametric studies that were conducted to develop guidelines for the design of superplastically formed sheet metal components. The MARC finite element code was used to construct models of a tray geometry for a range of sheet thicknesses, die geometries, and friction coefficients. Important model results included the final sheet thickness and the pressure history to maintain a constant maximum strain rate during the forming cycle. Methods are investigated that collapse these results to give design curves for the conceptual development of SPF components.

Session: F3-6 Room: CUB 224 **Time:** W1:00p-3:30p
Chairs: *M. Khaleel (PNL)*

Transformation Superplasticity Of A Whisker-Reinforced Titanium Matrix Composite

Schuh, C.A. and Dunand, D.C.
Northwestern University, USA

A titanium matrix composite reinforced with TiB whiskers was thermally cycled about the allotropic transformation temperature of titanium under an external stress. Enhanced tensile strains due to repeated transformation of the matrix are investigated as a function of the applied stress and considered in the framework of existing micromechanics-based models of internal-stress superplasticity. The mechanical effects of partial phase transformation are examined for thermal cycles of varying amplitude. Under thermal-cycling conditions, an effective stress exponent of unity was found at low stresses, and superplastic tensile strains (> 100%) were recorded. Microstructural evolution during deformation is also discussed.

A Parametric Study Of Void Growth In Superplastic Deformation

Khraishi, T.A., Zbib, H.M. and Khaleel, M.A.
Washington State University, USA

Substantial void growth in metals constitutes a problem in many industrial operations that utilizes superplastic deformation. This is because of the eventual and probable failure of the material due to such growth. Hence, there is a need to study void growth mechanisms in an effort to understand the parameters governing it. In this work, numerical and experimental studies of void growth, and the parameters that affect it, in a super-plastically deforming (SPD) metal have been performed. In the numerical studies, a 1• 2 thin plate (i.e. plane stress conditions) of a viscoplastic material with pre-existing holes has been subjected to constant tensile strain rates. The stress-strain solutions were obtained using the finite-element method. The experimental were performed under similar conditions to the numerical studies and provided for qualitative comparison. The parameters affecting void growth in SPD are: m (the strain-rate sensitivity), hole size (i.e. diameter) and the number of existing holes. The results showed that increased m values produced strengthening and decreased the rate of void growth. In addition, larger initial void size (or, equivalently, a larger initial void fraction) had the effect of weakening the specimen through causing accelerated void growth. Finally, multiple holes had the effect of increasing the metal ductility by reducing the extent of necking and its onset through diffusing the plastic deformation at the different hole sites and reducing the stress concentration. The numerical results were in good

qualitative agreement with the experiment and suggested the need to refine existing phenomenological void growth models to include the dependence on the void fraction.

Constitutive Modeling of Deformation and Damage in Superplastic Materials

Khaleel, M.A.
Pacific Northwest National Laboratory, USA, and
Zbib, H.M.
Washington State University, USA

Non-isothermal constitutive equations for superplastic behavior of modified 5083 aluminum alloys are presented. These equations describe the deformation mechanisms together with the localization effects and the evolution of the cavitation damage.

A Phenomenological Model For Aluminum Based Superplastic Materials

Booeshaghi, F., Garmestani, H. and Vaghar R.
FAMU-FSU College of Engineering, USA

A micromechanically based phenomenological model is presented here which predicts superplastic behavior for a wide range of strain rate and temperature for two different types of aluminum based superplastic materials (Al8090, Al7475). It is assumed that the total deformation is composite combination of grain boundary sliding accommodated by matrix deformation (dislocation climb and glide). Most models for superplasticity concentrate on the very narrow region were grain boundary sliding exhibits it maximum effect. The prediction should also include nonsuperplastic ranges for temperature and strain rate. The model proposed here is based on the mechanistic point of view originally proposed by Hart (1) that superplasticity occurs as a composite interaction of grain boundary sliding and matrix deformation. The matrix deformation is represented by a climb type model and for grain boundary sliding a viscous model proposed by Ashby and Verral (2). Using a recently developed microscopy techniques, Orientation Imaging Microscopy (OIM), this interaction has been investigated in the study of microstructural evolution in superplastically deformed Al-Li materials(3). The data can be reconstructed to produce grain boundary maps, which is a form of microstructure representation. The analysis of these maps revealed the complexity of the processes involved in the formation of high and low angle boundaries in superplastic materials. An attempt was made to correlate these misorientation data to the mechanical response of the superplastic material through a phenomenologically based model.

The material constants are assumed to be a function of the microstructure and these relationships are incorporated in the constitutive relationship. The main state variables for the model include grain size, a hardness value incorporating the dislocation density, Temperature. The model shows good predictions for 6-7 decades of strain rates.

1. E. W. Hart, *Acta Metallurgica* **15**, 1545-1549 (1967 September).
2. M. F. Ashby, R. A. Verrall, *Acta Metallurgica* **21**, 149-163 (1973 February).
3. H. Garmestani, P. N. Kalu, F. Booeshaghi, *Materials Science Forum* **243-245**, 569-574 (1997).

An Investigation on the Densification and the Sinter Forging Characteristics of Alumina - Magnesia Composites.

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Chokshi, A.H.
Indian Institute of Science, India, and
Raj, R.
University of Colorado at Boulder, USA

Superplasticity is the ability of a material to deform extensively under load without significant necking or cavitation. One of the major requirements for superplasticity is for a material to have a very fine grain size, typically less than 1 micrometer for ceramics. The possibility of forming ceramics superplastically offers a promising means of shaping them into complex shapes. This prospect is hindered largely by extensive grain growth that occurs during the final stages of sintering of ceramics. Although it is possible to obtain nanocrystalline powder, fully dense compacts have grain sizes typically greater than 1 micrometer. In the present work, alumina and alumina - magnesia composites were formed using the colloidal technique. Since magnesia hydrolysis in aqueous medium, the slurry was prepared in methanol and was pressure filtered under a constant stress of - 27 MPa. The green compacts were then sintered at temperatures of 1573, 1623 and 1673 K to study the effect of temperature on sintering and also to determine the activation energy for sintering. The green compacts were also sintered under uniaxial stresses without lateral constraints (sinter forging) to examine the effect of stress on densification. During sinter forging the shape change occurs by two processes - densification and creep. The contribution by each of these two processes was determined concurrently and stress exponent for creep and densification was evaluated. The microstructural investigation on the composite showed that the alumina-spinel boundaries are more stable energetically then other boundaries like alumina-alumina or spinel-spinel. This study shows the unique effect of boundary energy in the evolution and stabilisation of the microstructure.

The Characteristics of Deformation and Cavitation in Coarse-Grained Al-4.5Mg Alloys Exhibiting Superplastic-Like Behavior

Iwasaki, H., Hosokawa, H., Mori, T.
Himeji Institute of Technology, Japan,
Tagata, T.
SKY Aluminum Co., Ltd., Japan
Mabuchi, M.
National Industrial Research Institute of Nagoya, Japan, and
Higashi, K.
Osaka Prefecture University, Japan

The elongation-to-failures of two pure coarse-grained Al-4.5wt.% Mg alloys containing 0.09 and 0.2 wt.% Si have been investigated in temperatures between 613 K and 693 K and at strain rates of $1x10^{-4}$ s^{-1} , $1x10^{-3}$ s^{-1} and $1x10^{-2}$ s^{-1}. The elongation-to-failure greater than 350 % was obtained over a temperature range between 633 K and 673 K at $1x10^{-3}$ s^{-1} for both alloys. The maximum elongation-to-failures of 400 % and 380 % were obtained at 633 K at $1x10^{-3}$ s^{-1} for the 0.09 Si alloy and the 0.2 Si alloy, respectively. The elongation-to-failures at $1x10^{-4}$ s^{-1} and $1x10^{-2}$ s^{-1}, however, were decreased to about 250 % at all temperatures for both alloys. All specimens showed that their fractures were caused by local necking. Although the strain-rate sensitivity in the early deformation stage was about 0.33 for all strain rates, the strain softening was observed at $1x10^{-2}$ s^{-1} and no strain softening and hardening was observed at $1x10^{-4}$ s^{-1} and $1x10^{-3}$ s^{-1}. The plastic instability would be caused by surface roughening and internal cavitation during the deformation in addition to lack of strain hardening. The surface roughening was stimulated by increase in the strain and the grain size. The mean grain size of 50 μm was stable at temperatures below 650 K, and considerably increased with increasing temperature above 673 K for both alloys. The cavitation developed with increasing strain and Si content. The cavity volume fraction for the 0.09 Si alloy deformed up to a strain of 1.1 at 653 K at $1x10^{-3}s^{-1}$ was 0.7 %, whereas it was 2.1 % for the 0.2 Si alloy.

Symposium F4
Failure Modes in Heterogeneous Materials
Organizer
M. Zikry,
North Carolina State University, USA

Session: F4-1 Room: CUB 232 **Time:** T3:30p-5:30p
Chairs: *S. R. Kalidindi (Drexel U.) & M. Zikry (NCSU)*

Role-Specific Experiments for Dynamic Failure of Hybrid Composites

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Dynamic failure modes of layered structural systems consisting of ceramics, fiber-reinforced composites, and elastomers are considered. When subjected to a high velocity impactor, each constituent of such a system will have a different role in defeating the penetrator. It is often difficult to experimentally identify the failure mode of each constituent under controlled conditions. For a specific class of layered composites, we have sought to develop a technique to experimentally evaluate the failure mode of fiber-reinforced polymeric layers which used as the structural elements of hybrid-armor system, with a ceramic layer serving as the "armor". The lecture will present preliminary experiments and will provide a micromechanical model of the failure process.

Experimental Determination of Dynamic Crack Initiation and Propagation Fracture Toughness in Thin Aluminum Sheets

Owen, D.M., Zhuang, S., Rosakis, A.J. and Ravichandran, G.
California Institute of Technology, USA

An experimental investigation was undertaken to characterize the dynamic fracture characteristics of 2024-T3 aluminum thin sheets ranging in thickness from 1.63-2.54 mm. Specifically, the critical dynamic stress intensity factor was determined over a wide range of loading rates (expressed as the time rate of change of the stress intensity factor) using both a servo-hydraulic loading frame and a split Hopkinson bar in tension. In addition, the dynamic crack propagation toughness was measured as a function of crack tip speed using high sensitivity strain gages. A dramatic increase in both the critical dynamic stress intensity factor and the dynamic crack propagation toughness was observed with increased loading rate and crack tip speed, respectively. These relations were found to be independent of specimen thickness over the range investigated.

Plastic Deformation and Failure in an A359/SiC_p MMC under High-Strain-Rate Tension

Li, Y. and Ramesh, K.T.
The Johns Hopkins University, USA, and
Chin, E.S.C.
Army Research Laboratory, USA

The A359 matrix alloy and an F3S.20S composite (A359 aluminum alloy reinforced by 20% SiC particles) have been tested using the tension Kolsky bar. For purposes of comparison, a 6061-T6 matrix alloy and a composite consisting of 6061-T6 reinforced by alumina (Al_2O_3) particles were also tested with the same tensile facility. The fracture surfaces and the microstructure of specimens of each material were examined using SEM and optical microscopy. The experimental results show that the flow stresses of both composites were higher than that of their matrix alloys, while the composite fracture strains were lower than that of their matrix alloys. The fracture strains of both the 6061-T6 matrix alloy and the corresponding composite were much higher than those of the A359 matrix alloy and the F3S.20S composite. Both the A359 matrix alloy and the F3S.20S composite behaved in a brittle manner with no necking before fracture. Microscopic examination has shown that the tensile failure of the A359 matrix alloy and its composite are controlled by the microcracking of Si particles which formed in the interdendritic aluminum-silicon eutectic.

The Effect Of NaCl Concentration on the Low Temperature Hot Corrosion Behaviour of IN -738 and MAR-M-509

Allam, I.M.
King Fahd University of Petroleum and Minerals, Saudi Arabia

The influence of NaCl on the hot corrosion behavior of IN-738 and MAR-M-509 at 750 C has been investigated using Na2SO4/NaCl salt coating mixtures. The tests were performed under thermal cyclic conditions in air up to 150 cycle, one hour each. The results indicate that the rate of attack for both superalloys is directly proportional to the concentration of NaCl in the Na2SO4/NaCl mixtures. For both superalloys, exposures for up to 150 cycles using pure Na2SO4 and Na2SO2/ 1% NaCl salt coatings result in the formation of an outer porous layer of oxide mixture containing unreacted Na2SO4., below which a thin semi-continuous oxide layer exist along the corrosion product/metal interface. In either case, no pit formation, a typical feature of low temperature hot corrosion, has been observed. Increasing the concentration of NaCl to 25% in the salt coating mixture results in a dramatic increase of the rates of attack of both alloys. The corrosion morphologies were typical of low temperature hot corrosion, characterized primarily by the formation of large shallow pits filled

with oxides with virtually no sulfur present. At the bottom the pits, along the corrosion product/alloy interface, a thin zone enriched in sulfur is formed in both alloys. Basic fluxing, a model which involves the dissolution of protective oxides and their re-precipitation at the outer corrosion product/ gas interface has been proposed for the low temperature hot corrosion of both alloys in Na2SO4/25% NaCl salt mixtures during the propagation stages. The tungsten-rich phase in MAR-M-509 seems to enhance the hot corrosion attack during both the initiation and the propagation stages.

Effects of Temperature and Pressure in Dynamic Failure

Hanim, S. and Ahzi, S.
Clemson University, USA

It is well established that both temperature and pressure influence the process of dynamic plasticity and dynamic failure in materials. For instance, yield strength and brittle-ductile fracture transition are known to depend on temperature and pressure. The aim of this work is to propose a unified approach to introduce the pressure and temperature effects in most of the existing dynamic failure criteria and in constitutive modeling of dynamic plasticity. While this approach is physically based, its implicity makes it attractive for numerical implementation to simulate dynamic failure such as spallation. Results from this approach, as applied to different dynamic failure criteria to predict spallation, will be presented and discussed.

Session: F4-2 Room: CUB 232 **Time:** W9:30a-11:30a
Chairs: *S. E. Schoenfeld (US ARL) & M. Ortiz (Caltech)*

Three-Dimensional Simulation of Dynamic Decohesion in Layered Structures

Ortiz, M.
California Institute of Technology, USA

Compressive failure is often a design-limiting feature of thick laminated composites. However, a detailed understanding of the dynamic constitutive and fracture behavior of composites and associated failure modes, which is essential in interpreting and preventing impact damage, is yet to be developed. In particular, the early stages of delamination damage in composites are poorly understood at present. We have performed 3D numerical simulations of dynamic delamination experiments in thick laminated composites. A detailed theoretical understanding of failure processes in many composites is often hampered by the three-dimensional character of delamination. Thus, progress in the area necessitates the development of computational tools capable of following the progression of three-dimensional damage processes. The use of cohesive elements, which model the progressive decohesion of interfaces, provides a powerful tool for modeling crack nucleation and growth in three dimensions. The material parameters required in the constitutive and cohesive laws used in simulations are directly obtained from experimental data. Configurations analyzed to date include axisymmetric models of the Kevlar/aluminum impact test, as well as full 3D models of laminated plates subjected to impact.

Microstructural Failure Modes in Heterogeneous Materials

Zikry, M.A. and Jagannadham, K.
North Carolina State University, USA

An interrelated analytical, computational, and experimental investigation of the finite inelastic deformation and failure of crystalline materials has been conducted on length scales that range from the physical scale of dislocation densities to single grains. Three dimensional analytical and computational dislocation-density based multiple-slip constitutive formulations, in conjunction with carefully controlled TEM measurements and observations, have been developed to characterize intergranular and transgranular failure modes. The length scale between multiple-slip crystalline formulations and dislocation densities is bridged by coupling evolutionary equations, for the mobile and immobile dislocation densities, to a multiple-slip rate-dependent crystal plasticity formulation. The effects of different grain-boundary orientations, dislocation pile-ups, thermal and geometrical softening, mobile and immobile dislocation density interactions at grain-boundary interfaces and at crack-tips on the initiation and evolution of ductile and brittle failure modes have been investigated. Based on the present analysis, it is shown that dislocation pile-ups along grain-boundaries normal to the stress axis result in intergranular crack nucleation, and dislocation pile-ups along preferred slip-planes result in transgranular crack nucleation. These findings indicate that these nucleation sites, in combination with grain-boundary orientations and distributions, are the dominant mechanisms that control macroscopic crack propagation directions and planes.

Dimple Fracture Analysis Under Different Constraint Conditions

Kikuchi, M., Geni, M. and Muramatsu, A.
Science University of Tokyo, Japan

The dimple fracture test of A533B steel specimen is conducted by changing the crack tip constraint condition. It is found that the microscopic behavior is largely affected by the constraint condition. The fracture surface is observed using SEM, and the dimple fracture process is re-produced on the computer display. The number and diameter of dimples are also measured, and the effect of the constraint on these

values is recognized. Based on these observations, dimple fracture analyses are conducted using Gurson's constitutive equation. The fracture behaviors are obtained and the effects of the constraint condition on these phenomena are discussed.

An Adaptive Global-Local Analysis of Heterogeneous Materials with Evolving Microstructural Damage

Ghosh, S., Lee, K. and Moorthy, S.
The Ohio State University, USA

In this work, the Voronoi Cell finite element model (VCFEM) has been developed for damage initiation in heterogeneous microstructures. Two mechanisms viz. particle cracking and matrix cracking are considered for damage manifestations. The inclusion is assumed to be brittle, while the matrix is modeled as ductile with evolving porosity. An elastic constitutive relation is used for the inclusion, for which particle cracking is modeled by the Mohr's theory of maximum principal stress. To represent ductile failure, the matrix material is represented by a pressure dependent elastic-plastic constitutive relation. In particular the Tvergaard-Gurson model with void nucleation, growth and coalescence is used for modeling failure in the matrix.

An adaptive multiple scale finite element model is developed for elastic-plastic analysis of composite materials by combining asymptotic homogenization theory with the Voronoi Cell finite element model (VCFEM) and global-local computations. Asymptotic homogenization generates macroscopic material parameters and a local VCFEM analysis is invoked to depict the true evolution of microstructural state variables. Numerical examples are conducted to investigate the advantages of coupled multiple scale analysis over other unit cell and continuum based theories.

Session: F4-3 Room: CUB 232 **Time:** W1:00p-3:00p
Chairs: *K. T. Ramesh (Johns Hopkins) &*
G. Ravichandran (Caltech)

Modeling Dynamic Spall Failure in Metals

Ravichandran, G.
California Institute of Technology, USA, and
Tong, W.
Yale University, USA

Spalling in metals is a dynamic ductile failure phenomenon that occurs due to hydrostatic tensile stress produced by interaction of release or rarefaction waves. A model for spall failure of metals under plane shock wave loading based on dynamic void growth in viscoplastic solids [1] is presented. The model assumes the growth of voids and their coalescence in the spall plane under stress wave loading to cause failure. Void growth in the spall plane is modeled by hydrostatic tensile loading of an elastic/viscoplastic spherical shell. Simulations have been carried out for aluminum over wide range of loading rates and initial porosities. The geometry of the spherical shell determines the initial porosity. The release wave profile loading the spall plane is computed using a one-dimensional shock wave code and to determine the loading rates for the simulations. The combined effect of strain hardening and thermal softening appear to have minimal influence on void growth under conditions of spall. Inertia and rate sensitivity of viscoplastic materials have a strong effect on retarding the void growth and hence spallation. Porosity is identified as the damage parameter for spall and is computed as a function of applied stress and time. Spall failure is said to occur when the porosity reaches a critical value that leads to coalescence of voids. The results from the computations reveal the exponential nature of dependence of damage on time. Such dependence is generally postulated in classical spalling models. The spall strength is defined as the applied hydrostatic tensile stress when the porosity reaches its critical value. The dependence of spall strength on loading rate for pure aluminum is presented. The effects of inertia and rate effects on spall strength predictions are illustrated. The predicted spall strength is compared with experimental data as well as classical spall models.

[1] W. Tong and G. Ravichandran, "Inertial Effects on Void Growth in Viscoplastic Materials," Journal of Applied Mechanics, 62, 633-639 (1995)

An Investigation on Failure Waves from a Viewpoint of Phase Change

Chen, Z.
University of Missouri, USA

Based on recent observations in shock experiments on glasses, a new failure process has been suggested for a certain type of brittle solids, in which a failure wave propagates through a solid at some distance behind the compressive stress wave near but below the Hugoniot elastic limit (HEL). The peculiar character, that makes the failure wave seemingly different from usual inelastic shock waves (due to yielding or microcracking when the specimens are shocked beyond the HEL), is that the main quantities changed across the failure wave front are transverse stress for the increase in longitudinal motion (plate impact), or transverse motion for the decrease in longitudinal stress (in non-uniaxial strain cases).

With the use of a set of jump conditions (Chen, 1996), the concept of local dilatation has been used to explain the failure wave phenomenon observed in shock experiments on glasses (Chen and Xin, 1997). Although it is not clear whether geologic materials would exhibit the failure wave phenomenon, the concept of local dilatation implies that the similar phenomenon must exist in geologic materials because

their mechanical properties are usually pressure-dependent. To identify the initiation and evolution of a failure wave in plate impact experiments, it is assumed here that the phase change plays an important role so that a constitutive model with phase change should be developed for failure wave problems. Existing experimental data and sample calculations will be presented to demonstrate the proposed procedure.

Chen, Z., "Continuous and Discontinuous Failure Modes," Journal of Engineering Mechanics, Vol. 122(1), pp. 80-82, 1996.

Chen, Z., and Xin, X., "An Analytical and Numerical Study of Failure Waves," submitted for publication in International Journal of Solids and Structures1997.

Computation of Flexural Crack Width in Fibre Reinforced Concrete Members

Pandya, I.I., Shah, R.H. and Damle, S.K.
The M.S. University of Baroda, India

A method is proposed to determine the maximum crack width for fibre reinforced concrete flexural member by considering effect of percentage of fibres as well as span to depth ratio of beams. In recent years the control of crack width in reinforced concrete limit state design has become an important design consideration. A reasonably good estimate of width of crack becomes essential, because crack width is one of the prime criteria which designer has to satisfy. For serviceability of structure one has to keep the crack width and deflection within the permissible limit. Crack can be developed in reinforced concrete structures as the internal stresses exceeds permissible tensile strength of concrete. Due to introduction of high tensile strength deform bars, the problem of control of cracking has become more complex. Based on the test results of this investigation and using statistical analysis of the results, equation given by ACI-318-89 Building code for estimation of maximum crack width for reinforced concrete flexural member is modified.

The Nonlinear Behavior of Trusses under Earthquake

Ovunc, B.A.
University of Southwestern Louisiana, USA

The investigation encompasses the behavior of the trusses from their linear elastic to nonlinear elastic, to nonlinear inelastic stages, through loading and unloading, up to their failure. Moreover, the natural circular frequency of the system changes when it undergoes from linear to nonlinear state. Thus providing information about the members which are passed to nonlinear states, and their locations. The offshore platforms, power transmission towers, bridges, can be considered as truss systems. In order to determine the behavior of a system undergoing all possible states, the system must be accurately modeled. For the accurate modeling of a structure: the external disturbances, support motions, etc., acting on the structure; all the components of the structure: the superstructure, if any; the structure itself: the substructure, as the foundation and the soil, must be taken into account with their proper characteristics, material properties and with the proper interactions of their components. Herein, the actual stress-strain variation for a material is expressed by a continuous function, in terms of the material characteristics, constant for a given material, and the strains, varying with the magnitudes of the external disturbances. The continuous stress-strain function takes automatically care of the variation of the stresses through the linear elastic to nonlinear elastic, to inelastic states during the loading and unloading. Moreover, stresses beyond their yield limit create the geometrical nonlinearity. For the geometrical nonlinearity, the strains are expressed in terms of the displacement and the curvature on the deformed shape with respect to Eulerian coordinate axes systems, whereas, the displacements are expressed in terms of updated Lagrangian coordinate axes systems. The equilibrium equations or equations of motion are written for an infinitesimal element on the deformed shape. The dynamic responses are determined by linear acceleration method. Within a time increment, the effect of nonlinearities are included by an iterative process, which requires the linearization of the equations of motion. The equations of motion are linearized by writing the displacements which appear in the stress-strains function as the sum of the total displacements up to this iteration, plus the infinitesimal displacements of this iteration. Then expending the stress-strain functions in to two parts. One part, containing the total displacements of the previous iterations and the second part, containing the displacements of the present iteration. The software, STDYNL*, is modified to include the new formulations. The results of illustrative examples obtained by the new formulation are compared with those of previously obtained.

Session: F4-4 Room: CUB 232 **Time:** W3:30p-5:30p
Chairs: *A. Abdul-Latif (Paris 8 Université)*
M. Zikry (NCSU)

The Gigacycle Fatigue of Nickel Base Alloys

Bathias, C. and Bonis, J., C.N.A.M., France

In order to predict fatigue crack propagation at very long life a piezoelectric fatigue machine was built in our laboratory. This driver is able to fail specimen at 10^{10} device cycles and to determine thresholds until 10^{9} mm/cycles. The originality of this machine stays in the possibility to apply simultaneously to a specimen a constant tension effect and longitudinal ultrasonic

vibratory effort with adjustable amplitude. That is to say R ratio can varied from -1 to 0,9.

It appears that the fatigue thresholds are about the same in conventional fatigue and in resonant fatigue if the computation of the stress intensity factor K is correct. But there is a very large difference between the endurance limits at 10^6 cycles and 10^9 cycles. It means about 10% for steels and 30% for aluminum and nickel based alloys.

To improve the relation between thresholds and fatigue limits, the gigacycle fatigue is studied in a Ni alloy got by powder metallurgy with two sizes of inclusions. The testing temperature is 450°C. The first conclusion is that there is not any infinite fatigue limit until 10^9 cycles. The second conclusion is a possible correlation between the fatigue limit and the threshold at R ratio =0. This relation is much more improbable for R = -1 because an incubation phenomena exists around an inclusion or a porosity loaded at low stress level.

Engineering Fracture Mechanics - Vol. 56, n° 2, pp 255-264, 1997

Influence of Cold-Working and Aging Heat Treatment on Strength and Ductility

Kalidindi, S.R., Shaji, E.M. and Doherty, R.D.
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MP35N (35% Co, 35% Ni, 20% Cr, and 10% Mo) is a superalloy that exhibits a remarkable combination of high strength and high fracture toughness. This alloy derives its strength mainly from two processes - cold work and a subsequent aging heat treatment. This study examines the influence of the amount of cold-work, imposed in the drawing and the rolling processes, and the subsequent aging heat treatment on the strength and ductility (which is also an indicator of toughness) of this alloy. It was found that high levels of cold-work followed by the aging heat treatments resulted in a drastic drop in the ductility of the alloy. This drastic loss of ductility was correlated with appearance of macro-scale shear bands in the samples. The physical origin of these localized shear bands is investigated in this paper. Furthermore, this study established a processing window for MP35N (in cold-drawing and cold-rolling processes) where the aging heat treatment provides the desired increase in the strength without adversely influencing the ductility of the alloy.

Anisotropic Viscoplasticity in Rolled Aluminum Plate: Experiments and Simulations

Miller, M.P., Gunawardane, H.P. and Barton, N.R.
Cornell University, USA

Flat rolling produces metal plate with distinctly anisotropic material properties. Depending on the reduction, the in-plane yield strength and strain hardening character can vary significantly as the loading direction is varied in the rolling plane. In this paper we present experimental results of tensile tests conducted on rolled 7075-T6 aluminum plate (25 mm thickness). The specimens were extracted at various orientations in the rolling plane and then deformed to failure. Due to the processing history (hot-rolled, then tempered) the main source of the in-plane initial yield anisotropy is the rolling-induced crystallographic texture as manifested as differences in the ratio between the macroscopic stress and the average slip system hardness (the average Taylor factor). Anisotropic strain-hardening behavior, however, may be more indirectly linked to the texture and the Taylor factor through the shearing rate-dependent evolution of the slip system yield strengths. We explore these issues by simulating the experiments using an elasto-viscoplastic continuum slip polycrystal plasticity model. The orientations of the crystal aggregate were initialized with the rolling texture. The slip system hardening parameters were fit by correlating the tensile test data in the rolling direction. Issues related to anisotropic yield and strain-hardening were then explored as we attempted to predict the data from tests conducted in other straining directions. Finally, the ramifications for cyclic plasticity are discussed.

Inhomogeneous Texture Evolution During Explosive Forming

Schoenfeld, S.E.
Army Research Laboratory, USA

A description for the strain-rate and temperature dependent behavior of pure tantalum (Ta) at large strains is developed. An integral part of the model will incorporate the kinematics of crystallographic slip and thus, the rotation of single crystals within the material, so as to reflect the evolution of anisotropy as a result of the applied mechanical deformation. Such deformation is accommodated via bulk dislocation motion and governed by interactions that may or may not be thermally assisted. The model represents each discrete slip system as a single facet in a multisurface plasticity theory which is well suited to high-rate numerical methods (explicit integration schemes). A formulation of this type allows for the complete kinematic decomposition of macroscopic material rotations and the rotations of single crystals due to motion through the lattice. Implementation of the model within an explicit finite element analysis will resolve the effects of anisotropy and inhomogeneous texture evolution during explosive forming processes.

Study of the Local and Global Responses of Heterogeneous Polycrystals under Non-Proportional Cyclic Loading

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Université Paris8, France
Saanouni, K.
Université de Technologie de Troyes, France

A micromechanical model of rate-dependent plastic behavior which was recently proposed by the authors for FCC heterogeneous polycrystal, is examined using small strain theory. In this model, the inelastic behavior is modeled at the crystallographic slip system scale. At this level, the inelastic flow of polycrystalline structures is a manifestation of their heterogeneous deformation pattern principally influenced by the presence of microstructural inhomogeneities. Consequently, the microstructure heterogeneities profoundly affect the overall material strength and response. As an approximation, the granular elasto-viscoplastic strain rate is assumed to be uniform in each grain. The elastic part is treated at granular scale supposing to be uniform, isotropic and incompressible. Further, the intergranular heterogeneities, resulting principally from grain boundaries, is neglected. The transition from the single to polycrystal response is performed by classical averaging procedures. The anisotropy effect due the kinematic hardening is naturally described by the self-consistent interaction law.

The behavior of the polycrystal under non-proportional cyclic loading is of particular interest of this work. The model is used to describe the flow stress of the polycrystal under various out-of-phase angles (0°, 30°, 45° and 90°). Simulations are also conducted using other complex biaxial loading paths like butterfly and cruciform. An aggregate of 200 grains are systematically used for all these numerical simulations.

Macroscopic responses under such conditions are recorded and carefully analyzed. From the supplementary hardening point of view, it is found that this phenomenon is considerably influenced by the type of the loading path. The means that the greater the value of out-of-phase angle, the greater is the supplementary hardening, i.e., 90° out-of-phase gives the maximum hardening value in this condition. On the other hand, for more complex loading paths (like butterfly), the supplementary hardening becomes more important than that of 90° out-of-phase. The obtained results are shown to be, qualitatively, in good agreement with several experimental results available in the literature.

In order to elucidate the effect of these loading conditions on the local responses of the polycrystal and vice versa, some microscopic responses are recorded and then discussed. It is obvious that the transgranular plastic slips are highly localized in some defined orientations. In fact, one can conclude that the accumulated plastic slip distributions with respect to the applied loading direction is principally governed by the type of the applied loading path.

Symposium F5
Inelasticity and Material Instabilities
Organizer
D. Bammann
Sandia National Laboratories, USA

Session: F5-1 Room: CUB 232 **Time:** M10:00a-12:00p
Chairs: *M. Lusk (CO School of Mines) &*
K.T. Ramesh (Johns Hopkins)

On a Modulated Energy Function for Modeling Recrystallization and Grain Growth

Lusk, M.T.
Colorado School of Mines, USA

A phase-field model for recrystallization is presented which uses an orthogonal tensor to describe lattice orientation and degree of order. Grain boundaries are treated as regions of disorder across which the lattice orientation may change. A concept of energy modulation is adopted which satisfies material objectivity while still allowing an associated, regularized, energy function to explicitly depend on lattice orientation. Within a two-dimensional setting, only two equations need be solved: one for orientation angle and one for a scalar order parameter. Only one additional equation is required for three-dimensional simulations. This is a significant reduction in equations over the more standard approach that requires one equation for each orientation. An asymptotic analysis relates the theory to classical sharp-interface kinetics.

The theory is numerically implemented in both one and two dimensions in order to illustrate the existence and stability equilibrated structures. Both twist boundaries and fully three-dimensional lattice mismatches are considered. Plots are developed which give the grain boundary energy as a function of mismatch angle. An ad hoc dislocation substructure energy is also used to demonstrate how the associated driving force causes grain boundaries to move--an essential ingredient in simulating recrystallization.

Damage Localization Emerging from Microdamage Accumulation

Li, H.L., Gu, Y. and Bai, Y.L.
Chinese Academy of Sciences, China

According to the concept of statistical microdamage mechanics, we have derived a field equation of damage evolution. This equation, associated with the continuum equations, such as continuum and momentum equations, describes the evolution of mechanical field of a body with microdamage. With different numerical schemes, we carried out some numerical studies on the evolution of deformation as well as damage. The numerical results clearly show that in some cases damage localization can emerge under constant loading conditions, however minor inhomogeneity in initial damage is suppressed before then. The emergence of damage localization is in agreement with the prediction made by a criterion derived previously. The key in the criterion is the dynamic function of damage, which is the link between mesoscopic dynamics of micro-damage and its macroscopic description. The criterion indicates that the derivative of the dynamic function of damage with respect to damage overtaking the quotient of the function over damage (tangent of the dynamic function of damage becoming greater than its secant) signifies the emergence of damage localization. This is equivalent to a critical intrinsic Deborah number, the ratio of the interaction rate of microdamage to the rate of independently distributing nucleation. Moreover, inertial effect on damage localization is also discussed.

Modeling Adiabatic Temperature Changes Using Internal State Variables

Johnson, G.C.
University of California, USA,
Chiesa, M.L. and Bammann, D.J.
Sandia National Laboratory, USA

An internal state variable model for finite deformation inelasticity has been developed utilizing a multiplicative decomposition of the deformation gradient into elastic and inelastic parts. The theory is formulated with respect to the intermediate or stress free configuration, using Coleman-Gurtin thermodynamics. A scalar and a tensor state variable are introduced to represent dislocation density and distribution, respectively. Evolution equations are proposed based upon appropriate dislocation micromechanical models. In particular, the dislocation density hardens as a function of dislocation storage processes and recover due to mechanisms such as cross slip. Thermodynamic stresses are naturally defined as the derivative of the free energy with respect to the state variables. The product of these stresses with the time rate of change of the state variable naturally arise as source terms in the heat conduction equation. We investigate the effect of these terms for rapid loading cases where conduction can be neglected. Solutions for shear bands are compared with the usual assumption the 90-95% of the plastic work rate is generated as heat, and the remaining results in stored energy of cold work in the material.. In our model the effects of dislocation storage and recovery are naturally accounted for through the dissipation terms associated with the state variable evolution. The model prediction are also compared with the experimental results of Rosakis et. al., where the percentage of the plastic work which resulted in heat was shown to be a strong function of temperature.

An Experiment of Thermoplastic Shear Band for a High Carbon Low Alloy Steel

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and
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Thermoplastic shear bands have been previously studied because of their important in the forming processes at the high strain rates. In our study a high carbon low alloy steel was used to examine the mechanisms of shear bands. The effects of the size of second phase particles on the initiation and propagation of shear bands were considered. By using the way of different tempered temperatures and times the microstructures with different size of particle can be obtained. The rectangular parallelpiped on shaped specimens were purposed and designed, so that, when the specimen is subjected to an uniaxial compression loading, the middle section of the specimen is situated in plane strain state.

In order to study the patterns and properties of shear band for different high rates acting on the specimens, two kinds of loading devices with different loading speed were used in the study. One is a high speed hammer and the other is a light gas gun. Under the action of some loading devices, the average velocities of specimen's deformation, V are within the ranges of 10-20 m/s and 200-500m/s, respectively. The experimental results have shown that the shear band localization is still a main pattern which may lead to the failure of materials during the complex stress state. Under different loading speed, the patterns and properties of shear bands are not same. At relatively low loading rate, the band's pattern belongs to a deformed band type, but at relatively high loading rate, the shear band's pattern is not a deformed band. Transmission electron microscopy (TEM) was used to examine the interior and exterior microstructure of shear band. Some interesting results will be shown by using the tables and figures in the full text.

Acknowledgements: The support of this work through NSFC is gratefully acknowledged.

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Influence of Crystal Structure on the Dynamic Behavior of Materials at High Temperatures

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The rate dependent thermomechanical behaviors of OFHC copper, vanadium, and α-titanium have been examined using a recently developed experimental technique for the performance of high temperature, high-strain-rate experiments in the compression Kolsky bar. These three materials represent the three most common lattice structures for metals: FCC, BCC and HCP (respectively). Stress-strain curves are obtained for each material at strain rates of 4×10^3 s^{-1} and at temperatures ranging from 300 to 1100 K (27 to 800 C). Quasistatic thermal softening behavior is extracted from the literature for these specific materials and is compared with the new high strain rate data. It is observed that the rate of thermal softening is a function of the strain rate, with the strongest effects in BCC vanadium and HCP α-titanium. In addition, the differences in the high rate thermal softening behavior of the three different crystal structures are studied. Finally, the implications of these results on the constitutive modeling of BCC metals are examined. It is found that current constitutive functions are insufficient to describe the observed behavior. A new constitutive model is developed that is better able to describe the material response over the entire range of strain rates and temperatures. The model correctly captures not only the direct dependence of the flow stress on the strain, strain rate, and temperature, but also captures the coupling between the rate-dependence and the temperature-dependence.

Session: F5-2 Room: CUB 232 **Time:** M1:30p-3:30p
Chairs: *D. Bammann (Sandia) & D. A. Hughes (Sandia)*

Quantitative Representations of Dislocation Patterns from Experiments

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A truly predictive continuum level material model must account for the fine scale features of the deformation microstructure even though those features are numerically unresolvable in a finite element scheme. This task is nontrivial since the microstructure evolution is a result of the collective behavior of large populations of dislocations. Evidence for this collective behavior is found through quantitative post-deformation observations of the microstructure in the transmission electron microscope. Those results have shown that the dislocations arrange themselves into a long range pattern of dislocation boundaries that subdivides a grain into smaller volume elements at two size scales. Parameters that represent these microstructures include the spacing between

dislocation boundaries and the misorientation angle/axis pair across a boundary. Experimental results are discussed that show that the probability densities of dislocation boundary misorientation angles exhibit dynamic scaling for a wide range of materials, deformation modes and strain ranges. Furthermore, this scaling extends to the probability densities of the boundary spacings. Consequently the diverse probability densities are represented by one universal function. Within the scaling regime all of the material, deformation mode and strain dependence are represented by the evolution of the average values for the spacing and misorientation angle. Since the average value of the spacing is inversely related to the flow stress, this scaling law provides a direct link between the microstructure and the deformation.

*This work was supported in part by the U.S. DOE Office of Basic Energy Sciences, Division of Materials Sciences under contract no. DE-AC04-94AL85000.

Use of the Weibull Distribution to Model Variations in Ceramic DOP Results

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Since ceramics, as target materials, exhibit complex damage responses under rod impact, interpretation of penetration results is often difficult. When ceramics are used in bi-element ceramic/metal target configurations, a dynamic rod/target/target interaction can occur as well. Thus, in the latter case, interpretations can be most difficult. Our earlier work considered these possibilities, and, through analytic modeling of penetration, we can separate and evaluate the role of each factor. It was noted, however, the depth of penetration (DOP) test data for ceramic/metal targets displayed considerable scatter, even when dimensional tolerances and test conditions were controlled. In our previous modeling, we did not address the observed penetration variations.

The models of penetration suggest that target material densities and strengths are also dominate factors. For ceramic materials, in particular, the size of inherent flaws limits strength within the ceramic through Griffith's relationship. Flaws can vary in size, orientation and density within ceramics. Further, failure in a stressed ceramic body follows the weakest link theory that states that the most critical flaw determines failure at the lowest stress level that initiates crack growth. These notations lead to a size dependency of the ceramic effective strength called "size" effect. As a result, a Weibull distribution often represents the ceramic strength variations. This approach has become an important tool for predicting failure in ceramics and estimating design constraints in their use as structural materials. We have used the Weibull distribution to represent expected strength variations for ceramics and have explored such variations within the context of penetration. The current paper describes the application of the Weibull distribution into our penetration model and compares resulting calculations with experimental DOP data for AL_2O_3.

The Influence of Gradient Terms in the Evolution Equations on Dislocation Density Distributions

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Strain hardening in polycrystalline solids is due in part to the increase in dislocation density that accompanies plastic deformation. Dislocation densities become sufficiently high in most instances that the dislocations interact with each other in ways that impede their continued movement and that demand a higher level of stress to enable further deformation. Momentum balances performed on dislocations lead to evolution equations for the dislocation density that include gradient terms, weighted in the evolution equations by a coefficient that introduces a physical length scale into the theory. With these terms active in the model equations, hardening in a system that has a characteristic dimension of less than a grain diameter is influenced by the diffusional affect of the gradient term on the dislocation distribution. In this presentation, we discuss two applications of a plasticity theory in which the primary hardening variable is associated with the dislocation density whose evolution equation incorporates a gradient contribution. The first application is related to the hardening of material near the surface as a consequence of frictional traction applied on the surface. We focus on the influence that the gradient terms have on the depth of penetration of hardening below the surface.

The second application deals with the development of dislocation patterns when both mobile and immobile dislocation populations are modeled. Here we examine the relationship of the patterns to the characteristic dimensions of the deformation domain in a manner similar to Glazov and Laird.

Full Field Measurements of Shear Dominated Fracture in Dynamic Two Dimensional Punch Tests on High-Strength Metals

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Dynamic interferograms of adiabatic shear band initiation and propagation from the corner of a rigid die impacting a high strength steel plate are recorded and analyzed using a two dimensional model of a Dugdale crack initiating under the same conditions. The experimental method of using a thin plate allows

observation of the initiation and propagation of such shear failures. The simple experimental apparatus is discussed with some emphasis on the difficulties that arise. The analysis of the recorded interferograms focuses on measuring the stress intensity factor history and the average stress in the initiating Dugdale zone. Where earlier analysis used a quasistatic Dugdale crack model, these analyses are fully dynamic accounting for inertia in the material surrounding the zone. The results are compared to previously reported interferograms recording the initiation and propagation of a shear band from a notch tip under mode-II loading. The evolution of the stress intensity factor, with effects of the propagation of the Dugdale zone, is compared to predictions calculated using dynamic fracture mechanics concepts. It is seen that striking similarities exist between the two experiments and that the stress intensity factor can be used to characterize initiation under these conditions.

An Energy-Based Approach for Modeling Inelasticity

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It is energetically favorable for crystalline materials to develop complex dislocation networks in response to sufficiently intense mechanical loads. This process, however, is irreversible in that subsequent removal of the applied load does not cause the original state to be recovered. From an energetic perspective, this implies that the material has settled into a state for which the energy is, at least locally, minimized. These basic thoughts motivate the concept of an energy function that depends on dislocation density in two ways. The classic dependence of energy on dislocation content is simply based on the idea that an unloaded lattice with defects has a higher energy than its perfect counterpart. A nonclassical modulation of this basic dependence, though, results in an arbitrarily dense set of local energy minima. The finitely dense modulation may be thought of as a practical implementation of the essentially infinite set of actual minima observed in plastic deformation. Significantly, a correct choice of scaling between modulation amplitude and wavelength results in a material response that has a well-defined material behavior in the limit, as the modulation frequency becomes infinite. The result is a continuum level, thermodynamic description of plastic behavior that can be coupled to elastic and thermal processes. A similar approach was introduced by Abeyaratne, Chu & James [1] as a way of modeling the kinetics of tip splitting in martensitic twin structures. Such modulated free energies are referred to as wiggly energies.

In the present work, such a continuum thermodynamics model is proposed for the stress-induced development of dislocation substructure. Within a phase-field framework [2], dislocation density is tracked as a single, scalar variable. Dislocation forces are translated to a higher length scale and introduced as fields conjugate to dislocation density. The effects of such microforces on energy dissipation and irreversible thermodynamics are discussed. An energy function, dependent on elastic strain as well as dislocation density and its spatial gradient, is used to derive thermodynamic relations for the microforces. The balance of the microforces produces a kinetic equation for the evolution of dislocation density and the resulting equations exhibits kinematic irreversibility for sufficiently large deformations. Simple computational simulations are presented that illustrate such irreversibility and show that the approach can also capture the basic characteristics of rate-dependent inelasticity.

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Session: F5-3 Room: CUB 232 **Time:** M4:00p-6:00p
Chairs: *H. Zahrounii (U. of Metz) & A. D. Gupta (US-ARL)*

Micromechanics based on the Non-Riemannian Plasticity

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In this study, we propose a new microscopic approach to bridge the order gap lies between the dislocation theory and the classical crystalline plasticity theory based on the Non-Riemannian plasticity. The quantum field theory is introduced as the framework for extending the theory. The first part describes basic concepts of the Non-Riemannian plasticity which serves the most natural and substantial representation of dislocation and defect fields based on the differential geometry. Derivation of the field equation in strain and stress spaces, introduction of macro-micro interaction fields, and extension of the theory to the higher order space are briefly described, respectively. Secondly the paper discusses a rational description of collective behavior of dislocations which leads to pattern formations within a crystal based on the quantum field theory. The Ginzburg-Landau (GL) equation for dislocation densities is shown to be derived in the strict manner from the quantized Hamiltonian for a crystal body containing a large number of dislocations and dislocation dipoles. The derived GL equation gives the reaction-diffusion (RD) type differential equation, which has been reported to govern the periodic dipoler patterning such as shown in PSBs, when dislocation densities are taken as the order

parameters. Physical interpretation of the GL equation as well as pseudo-diffusion coefficient included in the equation is examined. Cell formation, which is composed of entangled dislocations, is also discussed from a topological point of view. Entanglement of dislocations can be expressed by the Gauss linking number, a topological invariant, and is closely related to the torsion tensor representing topological defects. Finally, T(3) and SO(3) gauge groups are introduced to provide the interaction between dislocation fields and the background field, i.e., a crystal lattice space having a translational symmetry. Relationship between the above field theoretical description and geometrical concepts in the Non-Riemannian plasticity is extensively discussed through the gauge field theory.

Modeling and Analysis of an Asymmetric Mine-Soil-Structure Interaction Problem

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An above-ground 2.44 m x 2.44 m x 15 cm rolled homogeneous armor (RHA) plate with a total mass of approximately 6350 kg located asymmetrically at a fixed horizontal 61 cm offset and a vertical 46 cm stand-off above a shallow-buried mine with an equivalent charge weight of 9.1 kg TNT and 15 cm soil overburden has been modeled using the CTH hydrodynamic code for simulation of mine detonation and propagation of explosive blast and soil debris and subsequent interaction leading to partial envelopment of the anvil plate which is employed as a momentum trap for a unique vertical ballistic impulse test facility currently under construction at APG.

The objective of this study is to obtain realistic simulation of explosive detonation, shock wave propagation in air medium and blast-soil-structure interaction under extreme loading conditions as well as generation of time histories of specified target output variables such as vertical and lateral displacements and velocities at critical tracer point locations along the median and back surface of the target as well as integrated vertical momentum trapped by the plate in addition to forcing functions such as pressure-time histories at specific locations of the target.

The computation was continued up to 2 ms or until time step instability occurred once the detonation products traveled around the bottom corners and partially enveloped the anvil plate. The tracer particles position data in 2-D under plane strain assumptions were used to calculate tilt angles due to plate rotation with respect to time to aid in the design of guide bars and mating guides in the experimental set-up and to avoid damage to the test fixture. The model allows parametric study of complex explosive-soil-structure interaction effects due to variation of explosive types and plate dimensions, standoff, types of soil and height of soil overburden as well as simulation of asymmetric transient loading on the ballistic pendulum anvil plate due to various off-axis locations of the mine relative to the target.

Adjoint Code Differentiation for Hydrodynamic Model Studies

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Expert use of a hydrodynamics code (hydrocode) for design or design-optimization purposes requires information about how some result (or response) will change when some code parameter is changed. This so-called sensitivity, can be used to determine which parameter or parameters are the most important. The sensitivity also provides the uncertainty of the response given the uncertainty of the parameter. For design optimization, the sensitivities are the gradient (or Jacobian) that determine the search direction for obtaining the optimum response. Previously, we have described an equation-based sensitivity technique used successfully for other applications, which is called Differential Sensitivity (DS). The system of partial differential equations describing the physical situation (the forward PDEs) are assembled, differentiated and adjointed, and the resulting adjoint PDEs are then solved using straightforward numerical operators. With an adjoint code, DS obtains the sensitivities of a single response to all of the problem parameters in only two computer runs (one run of the forward model and one of the adjoint code). One can also obtain sensitivities by changing parameters one at a time and form a finite difference sensitivity. This method requires at least N+1 forward model computer runs to determine sensitivities to N problem parameters. We have demonstrated that DS techniques provide accurate sensitivities for some parameters for single-material shock problems by comparison to the finite-difference method. We have seen, however, that our current DS techniques do not produce accurate values for all sensitivities, in particular, for problems with discontinuities such as multi-material problems. Here, we examine the source of these inaccuracies and expand our sensitivity capability by means of code-based Manual Differentiation (MD) and automatic differentiation (AD) techniques [ADIFOR (Automatic Differentiation of FORtran) and the Tangent-linear and Adjoint Model Compiler (TAMC)]. We describe the MD and AD techniques and apply them to the fitting of the data from a one-dimensional shock-physics experiment. We examine the relative run times using the various techniques for obtaining sensitivities to find that for this problem with 12 parameters that the adjoint technique requires less computer time than the forward methods. A larger number of parameters should produce a distinct run-time advantage for the adjoint methods.

Massively Parallel H-Adaptivity Applications

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Adaptivity of finite elements has been an area of strong research interest. The benefits to automated adaptation of spatial discretization offer computational advantages of increased accuracy of solution, reduced numerical error, reduced analysis time, and optimization of the finite element mesh. However, the application of adaptivity methods to large massively parallel analysis codes has been limited. We present our current efforts in this area. We have performed large-scale three-dimensional analyses using the H-Adaptivity method of mesh refinement. These analyses were carried out using the ALEGRA finite element code, a computer program, primarily designed for massively parallel computation of solid dynamic response of bodies. The code is written in the C++ language and utilizes object-oriented design. We have employed the object-oriented nature of the code to facilitate the design and implementation the H-Adaptivity algorithms.

Additionally, the massively parallel nature of the ALEGRA code, required development of parallel adaptivity capabilities and the ability to economically perform load balancing. The communication requirements between computational processors necessitated the development of algorithms to support synchronization of error metrics across processor boundaries. Substantial algorithmic development was required for maintaining valid communication boundaries in the presence of adaptation at processor boundaries. Finally, economic and consistent methods for load balancing have been necessary to shift the computational load off of processors with substantial refinement.

Furthermore, the development of refinement drivers appropriate for solid dynamic computation continues to be an area of active research. Much of the work in development of *a posteriori* error estimation methods has taken place for static mechanics or fluid dynamics problems and have had limited applicability for tracking stress wave propagation or propagation of detonation fronts. We will discuss the methods we have used to control the adaptivity process, assessments of the success of these methods, and the current direction of our work in this area.

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Asymptotic Numerical Method for Shells Using Nonlinear Constitutive Laws

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The aim of this work is to present an asymptotic numerical method (A.N.M.) to solve shell problems with plastic behaviour. This method allows us to search solution branches in the shape of power series [3]. In this way, we can transform the nonlinear problem into a set of recurrent linear problems which admit the same tangent stiffness matrix. Then, these latters are solved numerically by the Finite Element Method. The A.N.M. is efficient and easy to implement when the problem equations are written in quadratic form. Potier-Ferry et al. have shown how to make problems with strong non-linearities in this framework [4]. Then, we obtain a large part of the solution branch by inverting only one tangent stiffness matrix. When this method is applied in a step by step manner, it becomes a general and automatic method for seeking complex solutions [2].

In this study, we propose the application of the A.N.M. to shell problems which use nonlinear constitutive laws. Elastic unload is not taken into account; so, a total deformation theory is used. We consider a shell formulation proposed by Buchter et al. [1] which is based on a three dimensional constitutive law without condensation due to a vanishing stress in thickness direction. This extension is possible via the E.A.S. concept [5]. The resultant formulation is easy to implement in the A.N.M. context and well adapted to shell problems with large displacements and rotations. We propose three types of nonlinear constitutive laws. We show how to adapt these latters to the A.N.M. by keeping the rapidity and efficiency of the method.. Indeed, as the constitutive laws present some singularities, they are replaced by analytical expressions which allow us to apply expansions in power series. For the problems category considered in this work, it is shown that A.N.M. is **fast** (only few decompositions of stiffness matrices are needed compared to the Newton-Raphson method), **reliable** (automatic with adaptative steps) and **easy** to use.

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Symposium G1
Mechanics of Smart Structures
Organizer
H. Irschik
Johannes Kepler University, Austria

Session: G1-1 Room: CUB 212 **Time:** M10:00a-12:00p
Chair: *H. Irschik (Joh. Kepler U., Austria)*

Smart Materials and the Design of Solid-State Actuators

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Remarkable developments in the field of smart materials form the basis for the design of many novel actuators. Materials whose stresses and strains can be influenced by thermal, electric or magnetic fields offer the possibility to design solid state actuators for a wide variety of applications. Piezoelectric actuators for servo transducer applications in VCR head tracking systems, fast switching valves in fuel injection systems, adaptive microscope stages and deformable mirrors as well as ultrasonic motors are only first examples of the evolving technology of solid-state actuators. Optimistic estimates of the market for piezoelectric actuators and ultrasonic motors amount to more than $1 billion for the year 2000.

Although the final designs and applications of solid state actuators made from shape memory alloys, magnetostrictive materials, electrostrictive materials or piezoceramics may be quite different, their basic design principle is quite similar.

The present contribution will start with a survey on present and future applications of solid-state actuators and then concentrate on basic design principles for solid-state actuators made from smart materials. The generalized notion of an active material will be introduced: Different active materials will be compared with respect to their specific energy density and specific energy flow density. These characteristic material properties are extremely useful for the conceptual design of new actuators. Some basic design examples will be given. It will also be outlined how application specific demands concerning no-load stroke, blocking force and mechanical impedance of an actuator can be met.

Finally ultrasonic motors will be discussed in detail. Different types of linear and rotary drives will be compared with respect to their relative merits and potential applications. It will be shown that the no-load speeds, maximum thrust forces as well as the maximum mechanical power output of these motors can be derived from simple mental models of the systems' dynamics, making use of the previously defined characteristic properties of active materials.

The design methods and the results being obtained from the analysis of mental models have been validated systematically by experiments with commercial piezoelectric actuators and ultrasonic motors which have been tested in the actuator lab of the Heinz Nixdorf Institut.

Active Magnetic Stabilization of an Unsymmetric Rotor-Bearing System

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Hydrodynamic bearings supporting rotors of machines working under nominally constant transverse loads are expected to provide contactless support and smooth running of rotors in wide range of operating conditions. Without regard to the lubricating medium such rotor supports have an important disadvantage which consists in the fact that at high angular speeds the fluid film can transfer energy from the rotation to the transverse motion. This results in dynamic instability and self-excited vibration around a static equilibrium.

The mechanism of fluid flow-induced rotor instability is well recognized and the role of geometric and physical system parameters is explained. The problem is how to ensure stability under unexpected (accidental) growth of angular speed. An alternative approach is to apply magnetic bearings which find more and more applications as active elements of mechatronic systems. Their main feature is that they can support a rotor without any contact. It makes that wear and resistant torque are considerably reduced. Moreover, magnetic bearings are not sensitive to the angular velocity and can effectively support rotors at speeds of order 10^5 r.p.m. However, it is impossible to have a stable equilibrium position in a static field of attractive magnetic force. The electromagnetic bearing has to be controlled by a position feedback. The magnetic support has another disadvantage consisting in low radial stiffness which limits the applications to rotors of small transverse loads.

In the paper a method of antiwhirl control of rigid rotors supported on hydrodynamic bearings utilizing active magnetic actuators is developed. The hybrid hydrodynamic-magnetic bearings are applied to support a rigid rotor unsymmetric with respect to both geometric mass distribution and physical properties of hybrid supports. Hydrodynamic bearings provide the static load capacity of supports enabling the rotor to be considerably transversely loaded. The role of the magnetic forces is to stabilize the rotor behind its dynamic instability threshold corresponding to the fluid flow-induced self-excitation. Magnetic actuators of various configurations are used to generate additional radial forces contributing to the entire supporting force field. Two different control strategies are studied - one relating control signals to the current rotation speed, the other being based on detected velocity disturbances of the static equilibrium under constant in time transverse load. Both kinds of antiwhirl control are

found to be effective and can result in considerable increase in the critical speed of rotation. Rotor asymmetry generally introduces a stabilizing effect. Even in symmetric rotors asymmetry can be brought about by one-sided magnetic actuators with constant bias voltage. This opens a new chance for antiwhirl rotor stabilization in emergency situations.

Thermo-Visco-Elastic Analysis of High-Frequency Vibrations of Thin Plates

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The aim of this paper is threefold: (i) to present the fundamental equations of thermo-visco-elastodynamics in variational form, (ii) to deduce a higher order system of thin plate equations from the fundamental equations and (iii) to study a variety of special cases and also, the uniqueness of solutions, in the coupled plate equations. The paper begins with a survey of pertinent literature in Section 1, and then the three-dimensional fundamental equations are summarized for a non-polar, non-local and non-relativistic viscoelastic medium in Section 2. In addition, the fundamental equations are stated as the Euler-Lagrange equations of a unified variational principle.

The variational principle is modified and extended version of a recent variational principle due to the authors [Int. J. Solids Structures, 33, pp. 3937-3948 (1996)] in which a thermal field vector is introduced for the consistency in the fundamental equations. Section 3 deals with the geometry and the kinematics of thin plate of uniform thickness. All the components of mechanical displacements and the temperature increment are expanded into some series of the thickness coordinate of plate with a regular, finite and bounded region and without singularities of any type. In Section 4, following Mindlin's method of reduction, the variational principle together with the series expansions of field variables is employed to consistently and systematically derive the higher order system of two-dimensional plate equations in both invariant variational and invariant differential forms. The system of thin plate equations governs the extensional, thickness-shear, flexural and torsional as well as coupled vibrations of thin plate at both low and high frequencies by an appropriate truncation in the series expansions. Subsequently, attention is focused on certain special motions, geometry and materials in the equations of thin plate which are in agreement with those of some of earlier ones in Section 5. The uniqueness in solutions of the higher order plate equations is studied in Section 6. Some conclusions are drawn and, in particular, the temperature and/or time dependency of plate material is recorded and the effect of second sound is discussed.

Work supported in part by TUBA

Axisymmetric Dynamics of Composite Spherical Panels with Composite and Active Piezoelectric Stiffeners

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Application of piezoelectric actuators for reducing deformations and stresses in structures has been considered since the eighties. In particular, the concept of piezoelectric stiffeners for active control of flexible composite and sandwich structures has been investigated and proven feasible. The previous work of the authors (4th European Conference on Smart Structures and Materials, 1998) dealt with shallow spherical caps reinforced by piezoelectric and composite stiffeners using a replacement of the spherical coordinate system with plane coordinates. This restriction is lifted in the present paper where the spherical panel is characterized using the Donnell-Mushtari-Vlasov version of the Love shell theory.

The panel considered in the paper is reinforced by meridional and circumferential composite stiffeners. The former stiffeners carry closely spaced couples of piezoelectric actuators producing an active bending moment. The load includes a dynamic axisymmetric pressure and a thermal field that does not vary in the circumferential direction. The resulting global deformation is axisymmetric, as long as local asymmetric displacements between closely spaced meridional stiffeners can be disregarded. The analysis is conducted using a smeared stiffeners technique. The resulting equations of motion have variable coefficients and can be integrated numerically. A closed form solution is obtained for the panels with the meridional angle close to 90^0 using a Geckeler-type approximation.

Session: G1-2 Room: CUB 212 **Time:** M1:30p-3:30p
Chair: *M. Krommer & H. Irschik (Joh. Kepler U. Austria)*

Thermodynamic Derivation of Dynamic Boundary Value Problem and Heat Conduction Equation for Piezothermoelastic Materials

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The set of basic laws of thermomechanics of piezoelectric elastic materials includes the equations of motion formulated in terms of balances of momentum and moment of momentum, state equations and the two

laws of thermodynamics. The intent of the presentation is to show that the dynamic boundary value problem, state equations and the heat conduction equation for piezoelectric elastic materials are derivable from the first and second laws of thermodynamics. Also, a variational principle is derived for materials with time-dependent properties, for the case when the volume and surface forces are not "dead" and when the free energy of the material depends upon the temperature.

The derivation is carried out in the framework of the geometrically nonlinear mechanics of continua. The constitutive equations for the Cauchy stress tensor, heat flux, free energy and the entropy of the piezoelastic material are taken in the general form of functions of the following defining variables: spatial coordinate, temperature, the temperature gradient in actual configuration, the Cauchy-Green measure and material measure of the polarization. The latter is obtained in terms of the polarization vector and is a demand of the principle of material frame indifference.

The advantage of the approach is as follows. Since the boundary value problem, the boundary conditions and the variational principles are derived from the thermodynamics by using the objectivity principle, they satisfy *a priori* the above basic laws of nature.

A Reissner-Mindlin-Type Plate Theory Including the Direct Piezoelectric and the Pyroelectric Effect

Irschik, H. and Krommer, M.
University of Linz, Austria

This paper is concerned with flexural vibrations of smart plates. Smart plates are characterized by attached or embedded sensors and actuators whose actions are coordinated through a feedback control system. The concept of smart structures is put into practice by means of distributed actuators and sensors, usually realized by means of layers or patches made of piezoelectric material. Piezoelectricity is thus used to generate the distributed actuation and to perform distributed sensing of strains in the smart beam. The distributed nature of sensors and actuators in smart structures is highly desired from a control point of view, and promising practical applications have been reported in various branches of engineering.

In the present contribution, special emphasis is given to coupling between mechanical, electrical and possibly thermal fields, which is due to the direct piezoelectric effect and the pyroelectric effect. An equivalent single-layer theory is derived for the laminated plate, where the influence of shear and rotatory inertia is taken into account. For that sake, the kinematic approximations of Mindlin are applied. In extension to the existing literature, coupling of the deformation and the thermal field to the electric field is considered at the level of this first-order shear deformation plate theory. We show that coupling can be taken into account simply by means of effective stiffness parameters. This result is derived utilizing electric variational principles in combination with two appropriate approximations, namely neglecting the inplane components of electric field, and neglecting the inplane components of electric displacement, respectively. In the sense of the variational formulation, the two assumptions are shown to give basically the same formulations, where the difference is apparent in the effective shear stiffnesses only. In case of both assumptions, a parabolic distribution of the electric potential in the transverse direction of a piezoelectric layer is obtained. The resulting theory is of equal computational complexity when compared to the commonly used decoupled theory, but direct piezoelectric effect and pyroelectric effect are properly taken into account. The formulation thus should be of special interest in control engineering, where one seeks for both, an accurate and simple modelling of the structure.

Piezoelectric Vibrations of Composite Beams with Interlayer Slip

Heuer, R. and Adam, C.
Technical University of Vienna, Austria

Actuating piezoelectric effects in two-layer beams with interlayer slip are described in detail, where special attention is given to the identification of the piezoelectric actuation as a source of selfstress. It is demonstrated that piezoelectrically induced strains conveniently can be interpreted as eigenstrains acting in a background composite beam without piezoelectric actuators. The analogy between the piezoelectric effect and that of thermal strains, compare e.g. /1/, is utilized in the present paper, where a layer-wise first-order flexural theory is applied to two-layer beams of various boundary conditions. Bernoulli-Euler hypothesis is assumed to hold for each layer separately, and a linear constitutive equation between the horizontal slip and the interlaminar shear force is considered. One of the two layers is assumed to be made of a piezoelectric material. The governing sixth-order initial-boundary value problem is solved by separating the dynamic response in a quasistatic and in a complementary dynamic response, see /2/. The quasistatic portion that may also contain singularities or discontinuities due to sudden load changes is determined in a closed form. The remaining complementary dynamic part is non-singular and can be approximated by a truncated modal series of fast accelerated convergence. The solution of the resulting generalized decoupled single-degree-of-freedom oscillators is given by means of Duhamel's convolution integral, whereby the velocity and acceleration of the loads are the driving terms. Light damping is considered via modal damping coefficients. The proposed procedure is illustrated for piezoelectrically induced flexural vibrations, where the forcing function is of curvature type, and the

improvement in comparison to the classical modal analysis is demonstrated.

(1) Heuer, R., Irschik, H. and Ziegler, F., "Thermo-Piezoelectric Vibrations of Three-Layer Elastic Plates", Proc. 2nd Int. Symposium on Thermal Stresses and Related Topics, June 8-11, 1997, Rochester, N.Y., (R.B. Hetnarski and N. Noda, eds.), RIT 1997, 451-454.

(2) Adam, C., Heuer, R. and Jeschko, A., "Flexural vibrations of elastic composite beams with interlayer slip", Acta Mechanica **125**, 1997, 17-30.

Optimal Control of Plate Vibrations by Piezoelectric Sensors and Actuators

Kugi, A., Schlacher, K. and Irschik, H.
Johannes Kepler University of Linz, Austria

This paper is concerned with an infinite dimensional approach for the active vibration control of a plate by means of piezoelectric sensors and actuators. In order to control the excited plate vibrations, two different strategies will be compared. The first one is an extension of the suggestions of Kugi et al. 1997 and Schlacher et al. 1996, where we make use of spatially shaped distributed piezoelectric actuator and sensor layers. The pattern of the electrodes of these layers are designed within the controller synthesis in order to achieve a sensor/actuator collocation which optimally fits the control problem. In a second proposal we will investigate a special piezo patch configuration. For both cases, the spatially distributed and the patch configuration, the mathematical model is based on the fundamental relations of linear piezoelectricity and the deflection of the plate is described by an initial, boundary value problem. Since no damping is assumed, the mathematical model has the structure of an infinite dimensional Hamiltonian control AI-system. A nonlinear H-inf-design (Schlacher et al. 1996 or Kugi et al. 1997) extended to this special case of infinite dimensional systems is used to derive the optimal damping of the plate. Therefore, it is not necessary to approximate the system of partial differential equations by a finite set of ordinary differential equations to solve the problem of the design of the controller. Under certain observability assumptions of the free system the closed loop is asymptotically stable in the sense of Lyapunov. In this way, flexural vibrations which are excited by an axial support motion or by different time varying lateral loadings can be suppressed in an optimal manner. A numerical example serves both to illustrate the design process and to demonstrate the feasibility of proposed methods.

Kugi A., Schlacher K. and Irschik H., Optimal Control of Nonlinear Parametrically Excited Beam Vibrations by Spatially Distributed Sensors and Actors, Proceedings of DETC'97, ASME Design Engineering Technical Conferences, September 14-17, Sacramento USA, DETC97/VIB-4171, (1997).

Schlacher K., Kugi A. and Irschik H., H-inf-Control of Nonlinear Beam Vibrations, Proceedings of the 3rd International Conference on Motion and Vibration Control, Tokyo-Chiba, Vol.3, pp.479-484, (1996).

Transient Response of a Cracked Piezoelectric Strip under Arbitrary Anti-Plane Impact

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Tsinghua University, China

It is well known that piezoelectric materials produce an electric field when deformed and undergo deformation when subject to an electric field. Due to this intrinsic coupling phenomenon, piezoelectric materials are widely used as sensors and actuators in intelligent advanced structure design. When subjected to mechanical and electric stresses in service, piezoelectric materials can fail due to defects such as cracks, holes, etc. arising during their manufacture. Therefore, it is of great importance to study the electromechanical behavior of piezoelectric materials with defects. Moreover, it is known that the failure of solids is resulted from the final propagation of crack, and in most cases, the unstable growth of crack is brought about by the external dynamic loads. So the study of dynamic fracture mechanics of piezoelectric materials is much more urgent in the recent research. A finite crack in an infinite piezoelectric material under anti-plane dynamic electromechanical impact was investigated with the well-established integral transform methodology (Chen and Yu, 1997). Axisymmetric vibration of piezo-composite hollow cylinder was studied by Paul and Nelson (1996). The dynamic representation formulas and fundamental solutions for piezoelectricity had been proposed by Khutoryansky and Sosa (1995). The dynamic response of a cracked dielectric medium in a uniform electric field was studied by Shindo and his colleagues (1996).

In the experiment research as well as the real intelligent structures, piezoelectric specimen and components are of definite size, so the fracture mechanics of finite size piezoelectric material is much more interesting. In the present work, by using the well-established integral transform methodology, the dynamic response of stress and electric displacement around a finite crack in an infinite piezoelectric strip are investigated under arbitrary anti-plane impact. During the action of the dynamic loads, the crack was assumed static. The dynamic intensity factors of stress and electric displacement are obtained analytically as the solution of the Fredholm integral equation of the second kind, which would be obtained by well-developed numerical methods (Chen and Sih, 1977). The result for the cracked infinite piezoelectric material can be reduced from the present work provided the

width of the strip be infinite as well as the loads be the form of a Heaviside step function.

Session: G1-3 **Room:** CUB 212 **Time:** M4:00p-6:00p
Chairs: *V. I. Levitas (U. Hannover) & H. Irschik*

Numerical Simulations of Martensitic Phase Transformations in Plane Strain

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Colorado School of Mines, USA

Recently, Fried and Gurtin [1] developed a continuum theory, based on an order parameter, to model mechanically induced solid-solid phase transformations. The approach constitutes a regularized model that smears out physically sharp phase interfaces while still maintaining the same kinetics and kinematics, in an asymptotic sense, as its sharp-interface counterpart. This makes such a phase-field framework ideally suited to the numerical simulation of martensitic transformations driven by mechanical loading. The present investigation adapts the governing equations of [1] to martensitic phase transformations in plane strain. Attention is restricted to materials where the deformation at a point lies near a local minimum of the strain energy [2], so that the large transition strains and large rotations of the martensite variants can be captured. The equilibrium states of each variant are characterized according to the nonlinear theory of martensite [3]. In contrast to the sharp-interface theory, the phase-field paradigm allows for twin boundaries that do not satisfy the Hadamard condition, although such misorientations are energetically unfavorable. As a result, circular nuclei should tend to extend their boundaries along directions consistent with the Hadamard condition. Results will be shown which exhibit this behavior. Two twin variants are used to represent the products of a cubic-to-tetragonal transformation. While the twins are prescribed as elastically isotropic, it is argued that the effects of the distinct transition strains dominate any such material symmetry properties. This approach should also be applicable to the study of systems of twin variants. Moreover, the development of a habit plane in association with twin interaction with austenite could be simulated. These issues are of interest in this ongoing investigation.

1. E. Fried and M.E. Gurtin, Dynamic solid-solid transitions with phase characterized by an order parameter, Physica , 72 (1994) 287--308.
2. E. Fried and M.E. Gurtin, Semi-quadratic variational problems for multi-phase equilibria, Quarterly for Applied Mathematics, 54 (1996) 73-84.
3. J. Ball and R. James, Fine phase mixtures as minimizers of free energy. Archive for Rational Mechanics and Analysis, 100 (1987) 13-52.

Modelling, Analysis and Optimization of Smart Structures by the Finite Element Method

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In the development of smart structural systems design tools, such as general-purpose finite element codes, numerical simulation and prediction techniques must be developed in order to accurately and optimally design components and systems in industrial applications. In smart structures new problems arises due to the integration of active materials as actuators or sensors into the base material. The focus of the present paper is on piezoelectric ceramics as active components, which are mainly controlled by electrical fields and consequently, the governing equations to describe the behaviour of such highly integrated smart material systems have to extend to coupled electro-mechanical equations.

In the paper an overview about our finite element based tool for modelling and analysis of smart structures is given, which includes optimization procedures (e.g. for actuator/sensor placements) and allows also to include control strategies. The element library contains 1D, 2D and 3D finite multifield elements as well as special layered elements to simulate thin-walled structures with different layers of passive and active materials based on a layerwise constant shear angle theory. The options to simulate smart structures include static analysis, eigenvalue analysis and transient response. A substructure/superelement technique can be used in all cases.

In the design of a smart structure it is important to look at the global structural behaviour as well as local effects, such as fracture, delamination and damage due to mechanical and electrical loads, in order to design a damage tolerant material system with an optimal transfer behaviour between mechanical and electrical fields. Finite element analysis has also been used to study the additional influence of the electrical field at the fracture and delamination of smart piezoelectric material systems. Numerical experiments based on fracture criteria demonstrate that the electrical field can either aid or retard crack propagation depending on the direction of electrical loading.

In the paper several numerical results of the global behaviour of smart structures, such as active vibration damping and shape control, as well as local effects, such as fracture and delimitation, are presented and compared with experimental investigations.

Elastoplastic Materials with Martensitic Phase Transition at Finite Strains: Numerical Simulation

Idesman, A.V., Levitas, V.I. and Stein, E.
University of Hannover, Germany

Martensitic PT in elastoplastic materials is a complex thermomechanical process accompanied by the change of mechanical properties, transformation strain and a complicated distribution of local stresses and strains. We consider the instantaneous occurrence of PT in some volume based on thermodynamics, without introduction of volume fraction and prescribing the kinetic equations. There are only few known numerical approaches of such type for PT in elastoplastic materials for small strains. Usually transformation and plastic strains are finite, and a corresponding theory was developed in [1] with first numerical results in [2].

In this paper we present the problem formulation of martensitic PT in elastoplastic materials on a mesolevel for the case of small elastic strains, but finite plastic and transformation ones. The condition of nucleation includes - in contrast to known approaches - the history of local stresses variation in nucleus during the transformation process. The deformation model is based on the multiplicative decomposition of the total deformation gradient into elastic, transformation and plastic parts and the generalization of Prandtl-Reuss equations to the case of large strains and phase transitions. The structure of constitutive equations is similar for the cases of small and large strains.

The finite element solution algorithm is realized for the actual configuration with the true Cauchy stress tensor using the radial return technique. Numerical scheme and the algorithmic tangent stiffness matrix are similar to the case of small strains. Some modifications of the iterative algorithm related to the numerical integration of constitutive equations allow us to improve accuracy of solutions for large increments of external load (such modifications can be used for elastoplastic problems without phase transition as well). The problems of nucleation at shear-band intersection, appearance of a single martensitic plate and a single twin are solved and analyzed.

1. V.I. Levitas, Thermomechanical theory of martensitic phase transformations in inelastic materials. Int. J. Sol. Struct., Vol. 35, No. 9-10, 889-940, 1998.
2. A.V. Idesman, V. I. Levitas and E. Stein, Finite element simulation of martensitic phase transition in elastoplastic material at finite strains. In Computational Plasticity. Fundamentals and Applications. (eds. D.R.J. Owen, E. Onate and E. Hinton), CIMNE, Barcelona, 1323-1328, 1997.

Computational Evaluation of Poling Processes

DeGiorgi, V.G.
Naval Research Laboratory, USA

Design of smart materials is a complex process. As in the design of traditional structures, manufacturing and service loads are evaluated. While much work has been presented on design analysis methods for service loads, detailed evaluation of manufacturing induced stresses in smart devices is not commonplace. At the moment smart materials are shifting form laboratory based to production facility based. It is essential for fabrication processes to be designed which allow for the reliable production of smart materials. The use of established design tools, such as finite element methods, for the design of fabrication process is one way to help smart materials to transition to the production environment. Fabrication processes must be of equal concern to the designer as the end product service loads for this transition to be successful.

In this work one aspect of the fabrication of smart materials is examined. Poling, the process by which the piezoelectric effect is oriented to a preferred direction, is an integral part of the processing of ferroelectric materials for use in smart devices. Research on ferroelectrics has established that the poling process affects failure strength and other material properties. However the internal stresses developed during poling have not been examined. Successful poling must effectively establish the preferred direction for piezoelectric response while maintaining internal stress levels below critical values. Large residual stresses from the poling process, which may cause early failure of the device when combined with operating stresses, are undesirable. Any structural failures, such as cracks or other defects, resulting from high stresses induced during the poling process are unacceptable.

In this work competing poling processes for rectangular sections of a piezoelectric material measuring 125 x 10 x 5 mm are examined through a series of computational experiments. Internal stresses and electric fields in the section generated by the poling process are calculated using finite element techniques. Candidate poling processes are evaluated based on resulting field (and therefore magnitude of poling possible) and internal stresses.

Probabilistic Characterization of the Performance of Actively Controlled Smart Structures

Akpan, U.O. and Orisamolu, I.R.
Martec Limited, Canada

Smart materials and structural systems are increasingly attracting attention from the engineering community because of their importance in current and future high performance structural applications. As

these new structural systems emerge, there is an important need to have capabilities that can be employed for assessing their performance with reference to the primary functional requirement of structural integrity and control robustness as well as reliability. Furthermore, it is desirable to establish adequate performance metrics (which account for inherent or environmental uncertainties) that can be used as a quantitative basis for the comparative evaluation of various design options or for assessing the state of such systems that are already in service.

In this study, two measures that can be used for probabilistic characterization and assessment of the performance of actively controlled smart structures are developed. The framework is based on the use of the stochastic finite element method for the discretization of the parent (host) structure as well as the piezoelectric materials that are employed for sensing and actuation in the assembled system. The uncertainties inherent in the parent structure and the piezoelectric materials are propagated through the stochastic finite element model. This enables rational and realistic characterisation of the performance measures. The probabilistic models are based on the use of advanced reliability analysis algorithms which utilize fast probability integration algorithms that are robust and computationally more efficient than Monte Carlo simulation schemes. To facilitate efficient computation, an adaptive response surface methodology is employed for the approximation of the stochastic finite element response quantities. Example problems are used to illustrate the robustness and usefulness of the proposed methodology.

Session: G1-4 Room: CUB 212 **Time:** T9:30a-11:30a
Chairs: *K. Schlacher & H. Irschik (Joh. Kepler U. Austria)*

Active Vibration Control of Piezoelectricity Based Smart Structures, Theoretical and Experimental Results

Schlacher, K., Haas, W. and Irschik, H.
Johannes Kepler University of Linz, Austria

For the purpose of active vibration control, piezoelectric devices have shown great potential as actuators and sensors, because this technology allows space wise distributed sensors and actuators. This fact demands special control techniques to improve the dynamical behavior of smart structures built up with piezoelectric actuators and sensors. The first part of this contribution is concerned with the infinite dimensional approach for the active vibration control of a beam type structure with several spatially distributed piezoelectric layers. Here, the design of the spatial distribution of the sensors/actuators is considered as a part of the controller synthesis. Thus, it is possible to measure those integral quantities by means of the sensor layers that are required for the realization of the distributed feedback law. The mechanical model of the composite structure is obtained by using the theory of infinite Langrangian systems. The proof of stability for the proposed system is based on passivity which requires Ljapunov theory. Within this approach the hysteric characteristic of the constitutive relations of the piezoelectric material is taken into account. In the second part we investigate a infinite dimensional nonlinear controller design. An appropriate shaping of the sensor layers allows the measurement of the quantities required for the implementation of the proposed control law. In the third part we describe the experimental setup for the verification of our theoretical investigations. To realize the rather high sample rate, we propose a commercial digital signal processor (DSP) unit with additional A/D- and D/A-converters. This unit is supervised and programmed by the real time workshop of MATLAB. The experimental results show that this controller design leads to a satisfactory time behavior of the closed loop control system.

Kugi A., Schlacher K. and Irschik H., Optimal Control of Nonlinear Parametrically Excited Beam Vibrations by Spatially Distributed Sensors and Actors, Proceedings of DETC'97, ASME Design Engineering Technical Conferences, September 14-17, Sacramento USA, DETC97/VIB-4171, (1997).

Optical Fibre Techniques for Structural Measurements

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Optical fibre instrumentation offers a range of new measurement techniques which can be applied in monitoring mechanical structures complementing and expanding upon the potential offered by better established "conventional" instrumentation and measurement systems.

Traditionally measurements on mechanical structures have been made using devices such as thermocouples and strain gauges which (a) take a sample of the parameter field of interest at a specific point, and (b) are attached to the surface of the structure under test. Optical fibre instrumentation is available to perform analogous measurements but with the benefits that a single fibre can be used to multiplex together a large number of measurement points thereby obviating the need for interconnect. In addition optical fibres are mechanically and chemically more rugged than metallic systems and also are totally immune to electromagnetic interference and compatible with data transmission over very long distances.

Fibre optics does however enable different classes of measurements to be undertaken including so called distributed and quasi distributed architectures. The former enables a parameter field to be mapped as a linear function of position along an optical fibre with effective (but variable) gauge lengths of the order of

meters and extending, if need be, up to several tens of kilometers. For measuring temperature and strain fields the only equipment needed within the structure is a piece of perfectly standard optical fibre.

In quasi distributed measurements the system interrogates the average value of the parameter between specific points along an optical fibre. This measurement is particularly useful since it is capable of highlighting a fault between these two points and is more flexible in implementation than the fully distributed system.

The presentation will highlight the features of these various measurement architectures and then illustrate their potential. It will demonstrate that strain temperature, moisture ingress, hydrocarbon ingress or leakage and numerous other parameters can be readily accessed using distributed and quasi distributed architectures. In addition many of the systems which will be described have accumulated significant field experience and therefore have proven measurement capability.

Nonlinear Elastic Vibrations of Piezoceramic Shells Subject to Large Driving Voltages

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Dokmeci, M.C.
Istanbul Technical University, Turkey

ABSTRACT - Presented herein is a hierarchical system of two-dimensional equations so as to govern the extensional, thickness-shear, flexural and torsional as well as coupled nonlinear vibrations of piezoceramic shells subject to large driving voltages and large displacements. In the first part of the paper, the three-dimensional fundamental equations of piezoelectricity are summarized in a system of general convected (intrinsic) coordinates, and then they are expressed in variational form through an augmented version of a recent variational principle reported by the authors [Int. J. Engng. Sci., 34(7), pp. 769-782 (1996)] . In the second part, the geometry and the kinematics of a piezoceramic shell with regular, finite and bounded region are described and some preliminaries of surface geometry are recorded. Also, the components of mechanical displacements and the electric potential are represented by some series expansions of the thickness coordinate of piezoceramic shell of uniform thickness. Then, the hierarchical system of piezoceramic shell equations is systematically formulated by reducing the three-dimensional fundamental equations with the aid of the variational principle and the series expansions of field variables. The system of shell equations which is derived in both invariant differential and variational forms can be expressed in any particular system of convected coordinates most suitable to the shell geometrical configuration. Besides, the mechanical and electrical effects of higher orders can be taken into account as deemed desirable in any case under consideration. In the third part, considering a number of cases involving special motions, material properties and geometry, the system of shell equations is reduced to those of some of earlier studies. Moreover, the fully linearized system of shell equations is recorded and the uniqueness of its solutions is investigated by use of the logarithmic convexity argument. To assure the uniqueness of solutions, the sufficient initial and mixed boundary conditions are enumerated. Lastly, a unified numerical algorithm based on the method of moment is described and future needs of research are indicated.

Work supported in part by TUBA

Active Control of Plate Vibrations by Discrete PVDF Actuator and Sensor Segments

Gaul., L. and Stöbener, U.
University of Stuttgart, Germany

Acoustic enclosures of noisy machinery often consist of assembled plane plates. Measures of passive noise reduction such as damping layer can be effectively replaced by measures of active noise control. Laminated plates with PVDF coated segments which act as sensors or actuators allow to control the mode shapes and associated sound radiation. Such plates are excited by the noise source on principal and side paths by airborne and structure borne sound. Design rules of the PVDF segments are developed such that a selected number of modes can be identified and controlled. The use of symmetry and asymmetric conditions reduces the number of necessary PVDF segments and avoids the modal multilayer concept. The sensor signals corresponding to an operational mode are decomposed in their modal contents by adopting modal information from plate theory. These modes are controlled by the actuator segments in realtime for example with a PID controller. Experimental results validate the proposed concept.

Ionic Polymer-Metal Composites (IPMC) As Biomimetic Sensors and Actuators-Artificial Muscles

Shahinpoor, M.,
University of New Mexico

This paper discusses a number of recent findings in connection with ion-exchange polymer-noble metal composites (IPMC) as biomimetic sensors and actuators. These smart composites exhibit characteristics of both actuators and sensors. Strips of these composites can undergo large bending and flapping displacement if an electric field is imposed across their thickness. Thus, in this sense they are large motion actuators. Conversely by bending the composite strip, either quasi-statically or dynamically, a voltage is produced across the thickness of the strip between the

two conducting electrodes attached. Thus, they are also large motion sensors. The output voltage can be calibrated for a standard size sensor and correlated to the applied loads or stresses. They can be manufactured and cut in any size and shape and in particular in the form of micro sensors and micro actuators for MEMS applications. In this paper first the sensing capability of these materials is reported. The preliminary results shows the existence of a linear relationship between the output voltage and the imposed displacement for almost all cases. Furthermore, the ability of these ionic polymer-metal composites as large motion actuators and robotic manipulators is presented. Several muscle configurations are constructed to demonstrate the capabilities of these IPMC actuators. This paper further identifies key parameters involving the vibrational and resonance characteristics of sensors and actuators made with IPMC's. When the applied signal frequency is varied, so does the displacement up to a point where large deformations are observed at a critical frequency called resonant frequency where maximum deformation is observed. Beyond which the actuator response is diminished. A data acquisition system was used to measure the parameters involved and record the results in real time basis. Furthermore, reported in this paper are load characterization of such active polymer composites made with a noble metal such as platinum. The results showed that these actuators exhibit good force to weight characteristics in the presence of low applied voltages. Finally, reported are the cryogenic properties of these muscles for possible use by NASA in a harsh outer space environment of few Torrs and temperatures of the order of -140 degrees Celsius. These muscles are shown to work quite well in such harsh cryogenics environment and thus present a great potential as sensors and actuators that can operate at cryogenic temperatures.

Symposium G2
Phase Transformation in Active Materials
Organizers
A. Bhattacharyya
University of Alberta, CANADA
D. Lagoudas
Texas A&M University, USA
&
M. Taya,
University of Washington, USA

Session: G2-1 Room: CUB 212 **Time:** T1:00p-3:00p
Chairs: *M. Wuttig (U. Maryland) &*
K. Bhattacharya(Calif. Inst. Of Tech)

Computer Modeling of Mesoscopic Microstructure Formation in Coherent Phase Transformations

Khachaturyan, A.G.
Rutgers University, USA

The mesoscopic microstructure of active materials is usually formed by the self-assembling domain structure produced by the phase transformation. The common feature of these systems is that their mesoscopic domain structure and its evolution are driven by a reduction of the infinite-range multi-body interaction associated with accommodation of the transformation-induced strain in the martensitic crystals and/or the electric field in ferroelectrics. The formation of a domain structure and its rearrangement under applied stress or electric field results in the macroscopic shape change characterized by the transformation-induced strain. Response of the transformation-induced strain to the applied stress (or electric field) determines the active behavior of the material. To formulate a proper model of the domain structure, we should explicitly take into account the coherency strain energy and electrostatic energy of an arbitrary domain pattern. The system should "choose" itself the optimal evolution path to relax these energies. The most promising approach to this problem is a use of the Phase Field Kinetic Equations modified to include the infinite-range strain-induced interaction and the electrostatic dipole-dipole interaction. The computer simulations based on this approach are presented. They produce the realistic microstructures which are in excellent agreement with the electron microscopic observations. The origin of the pre-martensitic transformation and the effect of frozen-in structural defects on different aspects of the diffusionless transformation are discussed.

Martensitic Transformation in Constrained Films

Wuttig, M. and Roytburd, A.
University of Maryland, USA

A thermodynamic analysis is presented for the martensitic transformation in a constrained film upon cooling and heating. It is shown that this transformation proceeds with a variable selfstrain corresponding to a variable polydomain structure of the martensitic phase. The theory predicts a considerable shift of the transformation temperature interval and its broadening due to the constraint. Experimental studies of the stress evolution in NiTi polycrystalline films on Si substrates supports the principle thermodynamic conclusions.

Recoverable Strains in Shape-memory Polycrystals

Bhattacharya, K. and Shu, Y-C.
California Institute of Technology, USA

The shape-memory behavior of polycrystals can be significantly different from those of single crystals. A variety of materials display good shape-memory effect as single crystals; however, Nickel-Titanium is truly unique for the large recoverable strain in polycrystals. We will discuss a model for predicting recoverable strain in polycrystals and use it to identify reasons that make Nickel-Titanium special. We will also use it to identify materials with good shape-memory effect in thin film form.

New Materials with Unusually Large Magnetostriction

James, R.D.
University of Minnesota, USA

I describe recent research on magnetomemory materials: materials that combine ferromagnetism and shape-memory. The theoretical existence of such a material was evident from joint work with D. Kinderlehrer on the magnetoelastic behavior of TbxDy1-xFe2 (x about 0.3). I shall describe the evidence, together with recent work on a "constrained theory of magnetostriction" that is guiding the search (joint work with A. DeSimone and M. Wuttig). This line of research involves, in a crucial way, recently developed concepts in the mathematical modeling of materials. Some interesting examples of magnetomemory materials have been found (James/Wuttig) which exhibit, under relatively small fields, a magnetostrictive strain that is several times that of the best giant magnetostrictive materials.

Session: G2-2 **Room:** CUB 212 **Time:** T3:30p-5:30p
Chairs: *G. P. Carman (U. Calif.) & P. Rosakis (Cornell U.)*

Hysteresis and Stick-Slip Motion of Phase Boundaries In Dynamic Models of Phase Transitions

Vainchtein, A. and Rosakis, P.
Cornell University, USA

Shape-memory alloys undergoing stress-induced martensitic transformations exhibit a markedly hysteretic behavior in tensile experiments. The load-elongation curves from such experiments are nonsmooth and involves serrations. The serrations are accompanied by irregular, ``jerky' motion of the phase boundaries. In this work, we consider two one-dimensional dynamic continuum models for martensitic phase transitions. In both models, a bar with a nonconvex two-well elastic energy density is subjected to time-dependent displacement control boundary conditions. The wells in the elastic energy density represent two different material phases, austenite and martensite. Inertia is taken into account. In addition, viscous stresses, linearly proportional to the strain rate, provide energy dissipation. The first model also includes an interfacial energy term, modeled by a strain gradient term. In the second model, this term is omitted. Both give rise to nonlinear initial-boundary-value problems which are studied numerically and analytically.

Both models predict hysteresis which is caused primarily by metastability(presence of multiple equilibria) and phase nucleation. The hysteresis persists even when the loading rate is very low and viscosity effects are minor. We find that the model including interfacial energy results in smooth interface motion and small, non-serrated hysteresis loops, whose shape differs qualitatively from experimentally observed ones. On the other hand, in the model with viscosity only, the hysteresis loops in the load-displacement diagram are serrated and their shape is in qualitative agreement with experiments. In addition, the interface moves in stick-slip fashion. The serrations are caused by a succession of load rises during stick and load drops during motion of the interface.

Manufacturing, Testing, and Analysis of Thin Film NiTi Based Systems

Ho, K.
University of California Los Angeles, USA
Jardine, P.
Northrop Grumman, El Segundo, and
Carman, G.P.
University of California Los Angeles, USA

Shape memory thin film NiTi actuators are being considered for a variety of applications due to their exceptional properties. For example, NiTi based MEMS devices are being investigated for active flow control on a wide range of aerospace vehicles. Active Flow Control (AFC) represents an advanced concept for reducing drag, controlling flow separation, improving flight control effectiveness, and manipulation of wake vortex interactions in aircraft systems. While this illustrates the potential benefits associated with this relatively new actuator technology, manufacturing, testing and analysis for the thin film are not readily available. In this presentation we describe the ongoing work at UCLA in each of these three areas. A dedicated NiTi Ultra-High-Vacuum system is being used to sputter deposit the thin film onto a variety of substrates. Parametric studies indicate that processing parameters can be controlled to tailor the performance of the thin film for specific applications. Experimental tests are being conducted to evaluate the thermo-mechanical properties of the thin film including bandwidths, recovery force, and Youngs modulus. These are found to be dependent upon manufacturing parameters employed during the sputtering process. Simplified analytical models are being used to predict the displacements and bandwidths associated with different geometric configurations. The authors of this work are grateful for both the Air Force Office of Scientific Research (AFOSR) support under grant number F49620-98-1-0058 managed by Brian Sanders and Northrop Grumman DARPA / AFRL Smart Materials and Structures Demonstration - Smart Wing 2.

On Cross-Effects of Phase-Transformation And Plastification in Polycrystalline Materials

Oberaigner, E.R.
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Tanaka, K.
Tokyo Metropolitan Institute of Technology, Japan
Fischer, F.D. and Hein, G.
Institute of Mechanics, Japan

A specimen under external loading may exhibit a significant nonlinear behavior during a phase transformation due to temperature change. This behavior is known as "Transformation Induced Plasticity" (TRIP). Its basic mechanisms are accommodation and reorientation processes.

The authors proposed a unified thermodynamical concept [1] to describe the interaction of plastification and phase transformation and interpret the simulation results in the light of the basic mechanisms.

Starting point of the theoretical framework are the first and second law, from which a dissipation inequality is deduced. The dissipation rate is a function of the rates of the load stress, the temperature, and a set of internal variables, such as volume fraction of the new phase, transformation strain tensor, plastic

hardening, etc., as well as a conjugate set of thermodynamical driving forces. These are derived from the Gibbs free energy of the system.

Extremization of the dissipation rate under constraints (yield condition, transformation condition) leads to kinetic laws for the internal variables, which show clearly the coupling of phase transformation and plastification.

A symbolic-numerical computer program has been established [2], which takes as symbolic input the Gibbs free energy, the yield condition and the transformation condition, as well as a formula for the loading path. The numerical input is the set of material parameters and the initial conditions for the internal variables. The symbolic output are the kinetic laws for the internal variables, which are a set of nonlinear ordinary differential equations. The numerical and graphical output of their solutions are presented for a given loading path. Several cases (e.g. the classical TRIP test, biaxial loading, etc.) were simulated so far. The results are in good agreement with experiments.

[1]Fischer, F.D., Oberaigner, E.R., Tanaka, K., Nishimura, F.: Transformation-Induced Plasticity Revised, an Updated Formulation, to be published Int. J. Solids & Structures, 1997.

[2]Hein, G.: Masters Thesis, in preparation, Montanuniversität Leoben, Austria, 1997.

Session: G2-3 **Room:** CUB 212 **Time:** W9:30a-11:30a
Chairs: *M. Taya (UW) & A. Bhattacharya (U. Alberta)*

Thermomechanical Finite Element Analysis for Axisymmetric Shape Memory Alloy Structures

Boyd, J.G. and Capanu, M.
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Structural applications of shape memory alloys (SMA) are complicated by heat generation and conduction. Heat arises from the latent heat of transformation and the entropy production, and heat conduction from the structure is necessary for cyclic actuation. A closed-form structural analysis is impossible because the SMA is nonlinear and the equilibrium equation is coupled to the energy equation.

Therefore, the axisymmetric finite element analysis developed herein includes the (quasistatic) conservation of linear momentum, the conservation of energy, and SMA constitutive equations which include the latent heat and entropy production. The equations are cast in a nondimensional form.

Two problems are analyzed in detail:

(1) A hollow cylinder under longitudinal loading and inner pressure, with convection cooling applied to the inner boundary. The residual stresses, cyclic frequency and power of actuation are determined.

(2) A solid cylinder under uniform longitudinal loading with constant temperature boundary conditions on the outer boundary. This analysis is intended to simulate constitutive tests of SMAs. In fact, it has been experimentally demonstrated that SMAs exhibit an apparent rate dependence during ostensibly isothermal loading. It is demonstrated herein that this rate dependence can be due to the time dependence in the heat conduction from the specimen even if there is no time dependence in the SMA constitutive equations.

Simulated Superelastic Response of NiTi SMA Wires for Orthodontic Applications

Raboud, D., Faulkner, M.G. and Lipsett, A.W.
University of Alberta, Canada

Shape-memory alloys have begun to be used in orthodontic applications because of their properties (large elastic range, low modulus of elasticity and ability to deliver nearly constant forces over a wide range of deformations) which are ideally suited for orthodontic therapy. However, the detailed response of orthodontic appliances has been difficult to predict because the complex geometries of the wires coupled to the more complicated material response of the SMA. In order to develop a specific force/couple system necessary for the effective movement of teeth in orthodontic therapy, a more precise technique to simulate the response is required.

To affect a more exact simulation, the mechanical response of the NiTi SMA is modelled using a simple constitutive model which captures the essential superelastic behaviour of the wires. The solution to specific problems is done using an initial value iterative technique to converge to the appropriate boundary conditions. The advantage of the initial value approach is that it allows the material response to be evaluated at each segment of the appliance in turn rather than searching for the overall response.

The technique is applied to several appliance designs which have been used for conventional materials and allows the comparison of responses. The results indicate that the advantages of the SMA can be utilized to produce more ideal force/couple systems which will move teeth effectively.

Finite Element Modeling of Phase Transformation in Shape Memory Alloy Wires with Variable Material Properties

Bhattacharyya, A., Amalraj, J. and Faulkner, G.
University of Alberta, Canada

We revisit the problem of modeling the one-dimensional temperature distribution in a shape memory alloy(SMA) wire during a thermally induced phase transformation under constant load. Recognizing that the thermal and electrical properties of the wire, i.e. thermal conductivity, heat capacity, latent heat and electrical resistivity, change during the phase transformation and this change influences the evolution of the temperature field, we address the issue in the context of a specific boundary value problem of a SMA

wire heated electrically and cooled by convection. A Galerkin-based finite element method is implemented to model the one-dimensional(1-D) temperature distribution along the wire during phase transformation while the wire is taken through a complete cycle of heating and cooling. The implementation is done based on the following approach. The 1-D distribution in the temperature and the material properties is assumed to be known at the onset of a time increment. Assuming that the material properties remain unchanged during the time increment, the corresponding temperature increment is calculated. The new temperature distribution is used to calculate updated values of material properties, based on known evolution equations. These updated values are used for the next time increment. With this approach, the evolution of the temperature field during an entire cycle of heating and cooling is generated. The influence of the change in individual properties on the temperature field is then studied. We also compare the predictions of the model with some available experimental data.

Martensitic Transformation in Elastic-Plastic Materials Subjected to a Complex Loading Path

Wen, Y.H., Reisner, G., Fischer, F.D.
Leobeu, Austria, and
Tanaka, K.
Montanuniversität Leoben, Austria

A significant plastic deformation of an elastic-plastic material may occur even at a load level lower as the yield strength of the material if a solid state phase transformation induced by cooling takes place. This phenomenon is known since more than 70 years and is named "Transformation Induced Plasticity" (TRIP). An additional strain rate term $\dot{\underline{\underline{\varepsilon}}}_{TP}$ has been formulated being proportional to a coefficient k and the local average (mesoscopic) stress deviator $\underline{\underline{s}}$. k is a function of the transformed volume fraction, the yield stress of both, the parent and the product phases and the volumetric and shear components of the transformation eigenstrains [1]. Simplified micromechanical models have been established, confirming such type of relation.

However, in the last years experiments by a French group (Cailletaud, Pineau, Videau) and by one of the authors (Tanaka) have revealed that in the case of more complicated loading paths a somewhat different description is required. The French group proposed that $\dot{\underline{\underline{\varepsilon}}}_{TP}$ is proportional to $(\underline{\underline{s}} - \underline{\underline{\alpha}})$, $\underline{\underline{\alpha}}$ being a backstress tensor. A unified concept incorporating both plasticity and phase transformation based on thermodynamics of solids [2] confirms this proposal.

In this communication, we present a numerical model which enables us to describe martensitic transformation subjected to a complex loading path. The model is based on the finite element method and the unit cell technique. With the help of this model we investigate the development of a backstress $\underline{\underline{\alpha}}$ at the meso level, corresponding to the transformation process, and the associated mechanical behaviour under a complex loading path. The numerical results are compared to the experimental ones obtained from high alloyed steel. This steel transforms from austenite to martensite on cooling on air in the temperature range from 0°C to 200°C.

1. Fischer, F.D., Sun, Q.-P., Tanaka, K.: Transformation-Induced Plasticity (TRIP), *Appl. Mech. Rev.* **49**, 317-364, 1996
2. Fischer, F.D., Oberaigner, E.R., Tanaka, K., Nishimura, F.:

Micromechanic Modeling of Shape Memory Alloys and Their Composites

Taya, M. ,University Of Washington, USA
Lue, A. H.Y., University of Washington, USA
Tomota, Y., Ibaraki University, Japan
Inoue, K., University of Washington, USA

We are currently conducting several projects on smart materials and devices under the support of NSF, Boeing/DARPA and a small biomedical device company. Our main focus on these projects has been conventional and ferromagnetic SMAs. We have established the hierarchical modeling that can bridge the microstructure and mesobehavior of constitutive equations of a smart material as well as the macrobehavior of a composite structure that consists of the smart material as the key constituent. We reported the micromechanic modeling for a single crystal SMA in our previous paper. Where the model successfully predicted the microstructure of TiNiCu single crystal observed by Saburi et al. In this talk we will report the recent results of our study on polycrystalline SMA system by extending our previous model on a single crystal SMA where the microstructure of martensite phase was determined by minimizing the Gibb free energy (only mechanical part), ΔG_{mech}. In this study, we focus on the effect of temperature on the stress-strain curves of a SMA under both loading and unloading. The temperature range investigated are T=353, 361, 377 and 388 K, the results of the stress-strain curves at these temperature predicted by the present model are shown in Fig. 1, which indicates that superelastic behavior of the SMA can be observed at T=388K while shape memory effect at T=353K. Although there are no experimental data of the stress-strain curves of loading-unloading curves of Ti-40Ni-10Cu system at these temperatures, the trend that superelastic behavior occurs at higher temperature and shape memory effect at lower temperature is consistent with the experimental observation.

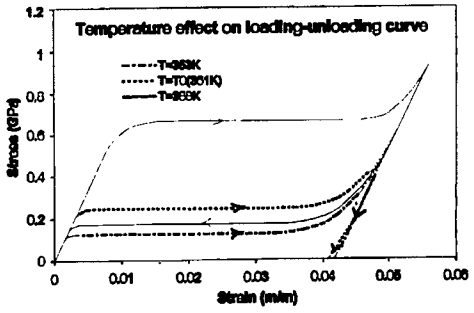


Fig. 1 Loading and unloading curves of Ti-40Ni-10Cu SMA predicted by the present model

Session: G2-4 Room: CUB 212 **Time:** W1:00p-3:00p
Chairs: *G. J. Weng (Rutgers U.) & A. Bhattacharyya (U. Alberta)*

Micromechanical Modeling Of The Transformation Induced Plasticity In Steels

Cherkaoui, M. and Berveiller, M.
LPMM, CNRS-ISGMP Ile de Saulcy, France

The Transformation Induced Plasticity (TRIP) phenomena accompanying the martensitic phase change in ductile materials is at the origin of development of steels with high ductility and ultimate tensile strength. In fact, the TRIP effect deals with at least two inter related inelastic strain mechanisms: plastic flow by dislocation motion and the inelastic transformation strain related with the martensitic phase change. In addition to the usual thermoelastic properties which may be assumed homogeneous for usual TRIP materials like steels, the plastic behavior of an austenitic-martensitic two-phase material appears strongly heterogeneous. According to the diversity of active strain mechanisms and the evolutive microstructure, various couplings have to be described. From a kinematical point of view, a volume element suffers a plastic strain in its austenitic state, followed by the instantaneous transformation strain according to discrete values of the possible set of transformation strains and plastic flow in the martensitic state. Beside the chemical part of the free energy, the elastic part is due to applied stresses but also to internal stresses generated by the incompatibilities of the whole inelastic strain field (plastic+transformation). These couplings lead to two well known effects:

The Magee effect (or orientation effect) corresponds to the orientation of the transformation (or to the variant selection) by internal as well as by applied stresses,

The Greenwood-Johnson effect (or accommodation effect) is related with accommodation by oriented plastic flow of austenitic and martensitic phases due to the local stress field inside both phases. Both effects are interacting and related by the internal stresses whose fluctuations are intra as well as inter granular. Intragranular stresses are related with the fluctuations of inelastic strains inside the austenitic grains while the intergranular ones come from the disorientation of austenitic grains and/or the polyphase nature of the representative volume element (austenite+ferrite+bainite for example). The aim of this work is to derive the behavior law for an austenitic single crystal (evaluation of intragranular stresses) from which the overall behavior of polycrystalline TRIP steels can be deduced using the self-consistent scale transition method (evaluation of intergranular stresses). The micromechanical modeling is based on the kinematics, kinetics and continuum-thermodynamic of the martensitic transformation.

Plastic strains of product and parent phases as well as the volume fractions of each martensitic variants are taken as the internal variables describing the microstructure evolution of the single crystal. From the derived Helmholtz free energy and dissipation, we obtain the driving forces acting on these internal variables according to the irreversible thermodynamic formalism. Comparison with experimental results for the stress-strain behavior of a TRIP steel and the corresponding evolution of the martensite content shows a good agreement.

Deformation Field Evolution During Transformation of Single Crystal SMA

Sun, Q-P.
The Hong Kong University of Science & Technology, China

The deformation field evolution during stress-induced martensitic transformation in single crystal CuAlNi shape memory alloys (SMA) under uniaxial tension is investigated by using high sensitive Moiré interferometry. The deformation patterns during superelastic martensite nucleation, growth and single interface propagation are obtained. The growth and reorientation of martensites are observed and measured habit planes are compared with the calculations based on the crystallographic theory of martensitic transformation. Several features of the deformation evolution are illustrated and fundamental issues regarding the nature of the *p-m* interfaces are discussed.

Interaction of Plasticity with Phase Transformation in SMA Actuators

Lagoudas, D.C. and Bo, Z.
Texas A&M University, USA

A generic form of Gibbs free energy for polycrystalline Shape Memory Alloys (SMAs) is first obtained in this presentation, by forming the increments of both elastic potential energy and Gibbs

chemical energy over a Representative Volume Element (RVE) with respect to an infinitesimal increment of martensite. A set of internal state variables, i.e., martensitic volume fraction, macro-transformation strain, and back and drag stresses due to both martensitic phase transformation and its interaction with plastic strains, are then introduced. Four primary mechanisms governing the transformation induced hardening effect are discussed. It is concluded that the back and drag stresses related to plastic deformation vary during phase transformation, even though the local plastic residual stresses are assumed to be constant. The evolution of plastic strains and the Two-Way Shape Memory effect (TWSM) with respect to cyclic thermally induced transformation cycles are then investigated. Motivated by experimental observations, evolution equations for the accumulation of plastic strains and plasticity related back and drag stresses, which govern the evolution of TWSM, are proposed. Finally, model predictions are compared with experimental data, and a procedure for the determination of material constants used in the present model with evolving plastic strains is discussed.

Influence of the Applied Stress on the Thermally-Induced Phase Transformation in Shape-Memory Alloys

Lu, Z.K. and Weng, G.J.
Rutgers University, USA

Martensitic transformation in shape-memory alloys is thermoelastic in nature, and is strongly dependent upon the applied stress and temperature. The objective here is to develop a micromechanical theory to determine how the martensite phase evolves without and with the applied stress during cooling, and how it recovers to the austenite -or parent - phase without and with the applied stress upon heating. In the martensite concentration, c_1, and temperature, T, space, such a recoverable process is represented by a closed loop. The theory aims at determining the precise path of each loop during the forward martensite and the reversed austenite transformation at zero and various levels of the superimposed stress. The micromechanical theory is developed first for single crystals by considering the microstructure of martensite as oriented thin plates using the theory of invariant plane-strain, each with a normal and shear component of phase transformation strain. Then the Gibbs free energy of the two phase system is established as a function of the applied stress and temperature by considering this microstructure. Based on the irreversible thermodynamics, this free energy provides the driving force for the martensitic transformation, and by considering the energy dissipation and creation of interface energy, the kinetic equation for phase transformation is established. The theory is then applied to a Ni-Ti single crystal under a pure thermal cycling, and then with a superimposed applied stress. The results show that the c_1 vs. T hysteresis loops noticeably move to the right on the temperature axis as the applied stress increases. As an extension to an SMA polycrystal, a 3-D microgeometry involving randomly oriented martensite plates is used to calculate the potential energy of the two-component system. The developed theory is then used to calculate the c_1 vs. T loops for a Cu-Al-Ni polycrystal at different levels of the applied stress. While quantitatively different from the single crystal case, the results also point to the strong applied-stress dependence of these hysteresis loops.

Session: G2-5 Room: CUB 212 **Time:** W3:30p-5:30p
Chair: *V. I. Levitas (U. Hannover)*

Global Criterion Of Phase Transition In Inelastic Materials Based On Stability Analysis

Levitas, V.I.
University of Hannover, Germany

According to theory of martensitic phase transitions in inelastic materials[1, 2], the local phase transitions criteria represent the equations for some parameters for the nucleus(nucleation criterion) or for the interface (propagation criterion). But even when they can be met, two solutions are possible [3]: first, the solution without the phase transitions, second, the solution with the phase transitions. It is suggested to use stability analysis for the choice of the unique solution. Using a postulate of realizability [1 - 3],an extremum principle for the description of a stable post--bifurcation deformation process for a finite volume of elastoplastic material with phase transitions is derived. The stable solution can be chosen using this extremum principle for the whole volume, which represents the global phase transitions criterion. Competition between two micromechanical mechanisms of inelasticity, namely dislocation plasticity and phase transitions is studied based on global phase transitions criterion. As an examples the phase transitions at shear band intersection and in spherical grain imbedded in cylindrical matrix are considered.

1. Levitas, V.I. (1997) Phase transitions in elastoplastic materials: continuum thermomechanical theory and examples of control. Part I and II. J. Mech. Phys. Solids, vol. 45, 923—947 and 1203--1222.
2. Levitas, V. I. (1998) Thermomechanical theory of martensitic phase transformations in inelastic materials. Int. J. Sol. Structures, vol. 35, 889--940.
3. Levitas, V. I. (1995) The postulate of realizability: formulation and applications to post--bifurcation behaviour and phase transitions in elastoplastic materials. Part I and II. Int. J. Eng. Sci., vol. 33, 921--971.

Micromechanics Modelling And Parametric Study In Microstructure Design Of SMA Composite

Sun, Q-P.
The Hong Kong University of Science & Technology, China

A quantitative microstructure-based modelling for the overall behavior of SMA composite is established and a parametric study on the role of each microstructure factors in the macroscopic behavior as well as in the internal stress and strain evolution of the SMA composites is performed. The SMA composite consists of ductile matrix and shape memory alloy (SMA) second phase inclusions with various shapes. The obtained results demonstrate several interesting deformation features of the new composite, which are expected to have potential applications in the future.

Theory of Pseudoelasticity Accounting for the Asymmetry in Tension-Compression of Shape Memory Alloys

Lexcellent, C., Rejzner, J.,
Institut des Microtechniques, France
Miyazaki, S.
University of Tsukuba, Japan and
Robinet, P.
Institut des Microtechniques, France

The thermodynamic theory of pseudoelastic behaviour of shape memory alloy (SMA) is generalized to include new observed effects as the asymmetry in tension-compression. Specific form of Gibbs potential is presented and new conditions for initiation of phase transformation are derived. They are expressed in terms of the temperature, second and third invariant of stress deviator. In a first stage, modeling of Ni Ti experimental results [1] for simple tension-compression and pure shear is performed. In a second stage, new biaxial experiments in the pseudoelastic range are in progress on Ni Ti thin tubes as tension (compression), torsion and internal pressure. It will permit to establish what is the effect of the isotropic part of the stress tensor on the phase transformation in reference of the paper of Jacobus et al (1996) [2].

[1] L. Orgeas, D. Favier (1996), "Non symmetric tension-compression behavior of Ti Ni alloy", J. de Phys. IV, C8, 605-610.

[2] K. Jacobus, H. Sehitoglu and M. Balzer (1996), "Effect of stress stage on the stress-induced martensitic transformation in polycrystalline Ni-Ti alloy", Met. And Mat. Trans. A., vol. 27 A, 3066-3073.

Thermomechanical Response of Polycrystalline SMAs under Cyclic Loading: Modeling and Experiments of Minor Hysteresis Loops

Bo, Z. and Lagoudas, D.C.
Texas A&M University, USA

A thermomechanical model for the hysteretic response of Shape Memory Alloys (SMAs) is proposed in this presentation by expanding a previous model developed by Bo and Lagoudas to include minor hysteresis loops and variable thermomechanical loading paths. The constitutive model for SMAs previously developed by Bo and Lagoudas is reviewed first, and a simplification for the case of fully trained SMAs with a stable major hysteresis loop is then presented. An evolution equation for the energy dissipation is proposed based on theoretical analysis and experimental observations. A connection between the Preisach hysteresis model and the present thermomechanical model is also investigated. The memory (wiping out) property for the present model is determined in a way similar to that of the Preisach model. Comparisons between the present model predictions and the experimental results show that the present model accurately predicts the minor loop hysteresis response of SMAs, even when such minor loops are close to the transformation start and finish points. Comparisons are also presented for various loading paths, including constant stress and spring loaded SMAs for complete and partial thermally induced phase transformations. Compared with the Preisach model, the present hysteresis model follows a thermodynamic formulation, which makes it easier to account for the effects of changing loading paths and two-way memory effect induced by cyclic loading. The developed numerical implementation algorithm can also be easily incorporated into other existing thermomechanical constitutive models, thus providing a general scheme for the modeling of hysteretic response of SMAs, based on physical parameters.

Temperature Induced Phase Transformation of An SMA Strip

Davis, A.K. and Sottos, N.R.
University of Illinois at Urbana-Champaign, USA

The shape memory effect is a diffusionless, solid-solid transformation induced by temperature change or application of external stress. Alloys such as Nitinol (NiTi) which exhibit the shape memory effect are capable of recovering up to 8% strain upon heating. The amount of recovery depends on the activation temperature, the initial deformation, and the percent of martensite phase that is present in the material. The large strain recovery properties have led to many applications of SMAs as thermally activated actuators for external shape, stiffness and vibration control.

In the current work, the thermoinduced transformation behavior of a thin SMA strip is investigated. A uniaxial strain of 6% is first applied along the axis of a Nitinol strip at a temperature below the martensite finish temperature (M_f). The strip is then subjected to heating along one boundary. As the temperature along the length slowly increases above the austenite start temperature (A_S) by conduction, the strip transforms from martensite to austenite. Moiré interferometry is used to measure the transient displacement and strain induced in the strip as it transforms. A sharp gradient in axial displacement is observed along the strip providing information on the location of the transformation front and how much of the ribbon has transformed. The displacement measurements also provide an independent set of data for comparison with theoretical predictions of the SMA transformation.

Symposium H1
Giga Scale Integration Technology: Device, Process and IC Design
Organizers
M.A. Osman, K. Mayaram
Washington State University, USA
O. Awadelkarim
Pennsylvania State University, USA
&
T. Yamada
NASA, USA

Session: H1-1 Room: CUB B1-5 **Time:** M10:00a-12:00p
Chair: *K. Mayaram (WSU)*

Low Power Image and Communication Chip Technologies (Invited)

Stork, J.M.
Hewlett-Packard, USA

The continuation of CMOS scaling will be driven to a large extent by demand for highly integrated, low power, embedded systems. Functionality and performance improvements will be directed to enhance the user interface and the communication capability, especially for consumer applications. The integration of logic and memory, digital and analog, image and RF functionality, at sub-0.25 um dimensions, presents significant challenges.

This talk will review activities at HP's ULSI Research Lab that address the challenges of developing and integrating sub-0.25 um CMOS technologies, including process development and simulation of devices, interconnect and lithography. The issues regarding the integration and scalability of various functions for "systems-on-a-chip", will be presented through examples of specific applications, such as RF CMOS and smart image sensors.

Low Power Mixed-Signal Silicon Systems: Applications, Architectures, Technologies and Design Tools (Invited)

Shenai, K.
University of Illinois at Chicago, USA

The demand in consumer electronics for portable computing and wireless communication devices is driving an evolution in microelectronics toward functional integration of digital logic, analog interfaces, and RF transceivers. The commercial success of these products depends on efficient battery power, and the low-power potential of functional integration is motivating system-on-a-chip (SOC) development. Ultra-low power operation requires a careful optimization of circuits and architectures and exploits process and device technologies that are difficult to integrate. This talk will discuss the architectures and circuit topologies, device technologies, and computer-aided design (CAD) tools relevant to the development of ultra-low power mixed-signal silicon systems.

Low Temperature MOS Microelectronics Opportunities and Challenges (Invited)

Deen, M.J.
Simon Fraser University, Canada

It is argued that low temperature MOS-based microelectronics should be considered as a viable option for future high performance digital electronic systems for giga-scale electronics. To quantify this argument, simple formulas are used to give an impression of the benefits of low temperature operation in terms of power, speed, energy and integration density. The possibility of a dynamic threshold MOS transistors with excellent characteristics at 77K will also be discussed. It will be shown that the low temperature operation allows for a large reduction in operating voltages of deep-submicron of a MOS transistors because of their improved subthreshold characteristics. This reduced operating voltages will significantly impact device density, device dimensions, and also device reliability problems that arise from large electric fields. It is proposed that 77K is an appropriate compromise temperature for systems that are silicon based. This temperature is also suitable for hybrid systems of MOS devices with III-V semiconducting or superconducting devices. To balance the presentation, some of the challenges and concerns such as thermal cycling, refrigeration, economics, testing and maintenance, of electronic systems in a 77K environment, will be presented.

Optimization of DRAM Sense Amplifiers for the Gigabit Era

Parke, S.
Boise State University, USA

The sense amplifier (SA) is perhaps the most critical circuit in a DRAM chip. It must reliably detect and amplify the small (<100mV) differential signal that appears on the bitlines following charge transfer from the storage cell capacitor. SA's must have high sensitivity, high performance, and very small area and layout pitch. As DRAM densities enter the gigabit era, there are three key SA design issues that must be resolved: 1)maintaining high performance despite decreasing array voltage, 2)maintaining sufficient sensitivity despite increasing effects of SA imbalances, and 3)reducing the chip area consumed by SA's despite increasing numbers of SA's per chip. To reduce power and maintain device reliability, the array voltage will be scaled to 1.5V and below. This severely degrades the sensing performance, because the threshold voltage

of the sense latch devices cannot be scaled as rapidly. Recently proposed preamplification techniques such as charge-transfer pre-sensing (CTPS) and charge-amplifying boosted sense (CABS) address this problem and will be presented in this paper. Sense amplifier devices typically suffer severe body-effect, raising their threshold, and delaying the onset and speed of sensing. Recent SA designs introduce dynamic control of the isolated wells containing the SA devices. The charge transfer well (CTW), body-synchronous, and super body-synchronous sensing schemes dynamically switch the wells synchronously with the sense lines to yield zero and even negative body-effect. In SOI DRAMs the dielectrically-isolated body has a greatly reduced capacitance, and can be switched with even lower power dissipation.

As DRAM density increases, the number of SA's per chip is also increasing to over one million on a 1Gb chip! This implies that for a given V_t distribution, a larger number of standard deviations (σ) must be tolerated for each successive DRAM generation. This growing problem has led to several designs that compensate for V_t mismatch. In the offset-compensating scheme (OCS), a current-mirror differential amplifier is added between the bitlines and SA which cancels ***all*** electrical imbalances. This achieves faster signal development and sensing, but increases the SA area by 70% due to the complicated current-mirror amp. Recently, an offset-trimming scheme has been proposed with both high speed and small area. Its performance is improved by 50% over an uncompensated SA, and its area penalty is only 13%. Several DRAM "gain" cells have recently been proposed. Instead of employing charge transfer, reading a gain cell causes a current to flow from the bitline to a power supply. There is no need for the SA to amplify the signals to full CMOS levels, thus improving its sensing speed. The number of cells attached to this SA can be greatly increased since the charge transfer limitation is removed. This can greatly reduce the number and area consumption of SA's on the chip. The new design concepts to be discussed in this paper will need to be combined and/or enhanced to enable reliable sub-1.5V sensing in multi-gigabit DRAMs of the future.

Session: H1-2 Room: CUB B1-5 **Time:** M1:30p-3:30p
Chair: ***M.A. Osman (WSU)***

Predictive Models for Semiconductor Device Design and Processing (Invited)

Meyyappan, M.
NASA, USA

The device feature size continues to be on a downward trend with a simultaneous upward trend in wafer size to 300 mm. Predictive models are needed m ore than ever before for this reason. At NASA Ames, a Device and Process Modeling effort has been initiated recently with a view to address these issues. Our activities cover sub-micron device physics, process and equipment modeling, computational chemistry and material science. This talk would outline these efforts and emphasize the interaction among various components. The device physics component is largely based on integrating quantum effects into device simulators. We have two parallel efforts, one based on a quantum mechanics approach and the second, a semiclassical hydrodynamics approach with quantum correction terms. Under the first approach, three different quantum simulators are being developed and compared: a nonequilibrium Green's function (NEGF) approach, Wigner function approach, and a density matrix approach. In this talk, results using various codes will be presented.

Our process modeling work focuses primarily on epitaxy and etching using first-principles models coupling reactor level and wafer level features. For the latter, we are using a novel approach based on Level Set theory. Sample results from this effort will also be presented.

The author acknowledges contributions from M. Anatram, B. Biegel, B. Bose, H. Hwang, and T.R. Govindan.

Simulation Needs for Ultra-scaled Silicon Devices (Invited)

Ravaioli, U.
University of Illinois at Urbana-Champaign, USA

Scaling of integrated devices beyond the 0.1 micron limit presents new challenges and fabrication costs of such magnitude, that a reliance on simulation predictions would be very desirable. However, standard CAD device simulation approaches are certainly inadequate to resolve the details of physical transport in semiconductor devices of extremely small size. Hot carrier transport, quantum effects and system granularity are some of the most prominent effects that must be addressed in advanced simulation models.

There are two possible paths to arrive at a realistic simulation framework. One way is to begin from the perspective of idealized ballistic quantum models for single carrier transport, valid at low temperature and/or low carrier density, and progressively included different levels of complexity for inclusion of scattering and particle interaction. Another way is to begin from semiclassical transport at the level of Boltzmann equation or Monte Carlo particle simulation, valid for relative large devices and try to extend the validity of the models by inclusion of some quantum features, by modification of the scattering models, and so on.

In the foreseeable future, silicon device scaling will concentrate on feature size ranging from 0.1 to 0.01 micron. Laboratories have already reported a number of working devices with gate length well into this range. Since the room temperature coherence

length of silicon corresponds to even smaller sizes, it is hoped that an extension of the available semiclassical models might be sufficiently useful and predictive to address the most urgent simulation needs.

This talk will present several case studies illustrating simulation issues for ultra-scaled silicon devices. First, a scaling analysis based on Monte Carlo simulation of conventional MOSFET structures in the 0.1 micron range will be presented. This will be followed by a discussion of devices realized with silicide contacts that require the inclusion of tunneling injection in a Monte Carlo simulation. Quantum models will be also discussed for the analysis of the limits of scalability in the third dimension transversally to the conduction channels, and for the simulation of some ultra-small memory device configuration.

Statistical Modeling from Case Files and Process Monitoring Data

Singhal, K. and Fisvanathan, V.
Lucent Technologies Inc., USA

Statistical device models are of great value in verifying the robustness of cutting edge mixed-signal designs. With such a model it would be possible to determine the standard deviations and correlations of the various performance metrics. Equivalently, it would be possible to determine the percentage of sample circuits that satisfy all the performance specifications, i.e., determine the parametric yield.

Most existing approaches to statistical device modeling assume the availability of I-V measurements on a large number of devices. Device model parameters are then extracted for each measured device using standard parameter extraction techniques. From this data base, the correlated distributions of the model parameters is determined and forms the basis of further statistical analysis.

Such an approach is however not practical in a production environment for the following reasons.

Device models that capture both nominal and extreme behavior are needed early in the life cycle of a process. It is possible to generate worst-case files early, since they are to a large extent based on process specs. At this stage it would be more appropriate to extract a statistical model from the case files.

A process typically shifts through most of its lifetime. Thus is may be necessary to update the statistical model at some regular interval. Requiring a fresh large set of I-V measurements in order to do this, is not a very efficient approach.

In this paper we describe an alternate approach to statistical modeling which fits in easily with existing modeling and process monitoring methodologies. We have currently applied the technique to the ASIM MOS model.

Essentially, we attack the problem on two fronts. First, we describe a technique for developing a statistical model based on worst-case files. Thus, as soon as the worst-case files are established (or modified) for a particular process, an associated statistical model can be immediately developed. Next, we address the issue of updating the model as the process matures. This is accomplished by basing the model on the data that is routinely collected to monitor the process. In both cases, the key statistical technique that is used is principal component analysis. The technique is well-established in multivariate statistical analysis and has been used in statistical MOS modeling. Our use of it is however novel in that we manage to extract significant statistical modeling information from very small data sets and existing process monitoring information.

The technique has been successfully applied to a 0.35 micron CMOS process. Further, since the statistical variations of the process are captured in a small number of independent principal components, we have also developed an accurate statistical circuit simulation technique based on Latin Hypercube sampling, that uses far fewer samples than would be needed in traditional Monte Carlo simulation.

Simulation of Ultra-Small MOSFETs Using a 2-D Quantum-Corrected Drift-Diffusion Model

Biegel, B.A.
NASA, USA
Rafferty, C.S.
Lucent Technologies
Yu, Z.
Stanford University, USA
Ancona, M.G.
Naval Research Labs, USA
Dutton, R.W.
Stanford University, USA

The continued down-scaling of electronic devices, in particular the commercially dominant MOSFET, will force a fundamental change in the process of new electronics technology development in the next five to ten years. The cost of developing new technology generations is soaring along with the price of new fabrication facilities, even as competitive pressure intensifies to bring this new technology to market faster than ever before. To reduce cost and time to market, device simulation must become a ore fundamental, indeed dominant, part of the technology development cycle. In order to produce these benefits, simulation accuracy must improve markedly. At the same time, device physics will become more complex, with the rapid increase in various small-geometry and quantum effects.

This work describes both an approach to device simulator development and a physical model which advance the effort to meet the tremendous electronic device simulation challenge described above. The device simulation approach is to specify the physical

model at a high level to a general-purpose (but highly efficient) partial differential equation solver (in this case PROPHET, developed by Lucent Technologies), which ten simulates the model in 1-D, 2-D, or 3-D for a specified device and test regime. This approach allows for the rapid investigation of a wide range of device models and effects, which is certainly essential for device simulation to catch up with, and then stay ahead of, electronic device technology of the present and future. The physical device model used in this work is the density-gradient (DG) quantum correction to the drift-diffusion model [Ancona, Phys. Rev. B 35(5), 7959 (1987)]. This model adds tunneling and quantum smoothing of carrier density profiles to the drift-diffusion model.

We used the DG model in 1-D and 2-D (for the first time) to simulate both bipolar and unipolar devices. Simulations of heavily-doped, short-base diodes indicated that the DG quantum corrections do not have a large effect on the I-V characteristics of electronic devices without heterojunctions. ON the other hand, ultra-small MOSFETs certainly exhibit important quantum effects that the DG model will include: quantum repulsion of the inversion and gate charges from the oxide interfaces, and quantum tunneling through thin gate oxides. We present initial results of 2-D DG simulations of ultra-small MOSFETs. Subtle but important issues involving the specification of the model, boundary conditions, and interface constraints for DG simulation of MOSFETs will be illuminated.

Session: H1-3 Room: CUB B1-5 **Time:** M4:00p-6:00p
Chair: *T. Yamada (NASA)*

Quantum-Dot Cellular Automata (Invited)

Porod, W.
University of Notre Dame, USA

We have recently proposed some ideas of using coupled quantum dots to realize both digital and analog computing elements[1]. Our scheme was inspired by recent work on nanometer-scale lithography in semiconductors which was permitted the construction of quantum dots which may be viewed as artificial atoms. This talk will review the work of the *Notre Dame Nano Devices Group* on the theory and modeling of such cellular arrays of coupled quantum-dot molecules.

We consider inhomogeneous arrays of quantum-dot molecules, where each molecule forms the basic unit in a cellular automaton-type array architecture. These cells (molecules) consists of four or five quantum dots in close enough proximity to enable electron tunneling between dots. Each cell is occupied by two electrons, the occupancy being simply determined by the voltage on relevant gate metal layers. Our modeling shows that control of the dot occupancy in the few-electron regime is feasible[2]. Coulomb repulsion between electrons in the cell results in a bistable ground state whose configuration is determined by the configuration of neighboring cells. The electrons tend to occupy antipodal sites in one of two ground-state configurations; we refer to these two states as states of +1 and -1 polarization. These two distinct charge configurations may be used to encode binary information. The response of a cell to the electrostatic effect of a neighboring cell is extremely nonlinear, tending to align it in the same state as its neighbor. This nonlinear response, coupled with the intrinsic bistability of the cell, plays the role of gain in conventional digital devices. Signal levels are restored at each stage leading to robust transmission and processing of information. We have demonstrated that logical gates can be constructed, and simple design rules permit the fabrication of any logic function.

1. C.S. Lent, P.D. Tougaw, W. Porod, and G.H. Bernstein, *Nanotechnology* **4**, 49 (1993); C.S. Lent, P.D. Tougaw, and W. Porod, *Appl. Phys. Lett.* **62**, 714 (1993); G. Toth, C.S. Lent, P.D. Tougaw, Y. Brazhnik, W. Weng, W. Porod, R.-W. Liu, and Y.-F. Huang, *Superlatt. Microstruct.* **20**, 473 (1996).
2. M. Chen and W. Porod, *Journal of Applied Physics* **78**, 1050 (1995).

Toward Sub-millimeter Scale All-Optical Switches for Ultrahigh Data-rate Applications (Invited)

Citrin, D.S.
Washington State University, USA

The coming generation of optical time-division multiplexed systems for telecommunications and other applications will operate in the 100 gigabit/sec range. Future-generation systems will operate in the terabit/sec range. Suitable optical switches remain one of the major hurdles to overcome before the deployment of these systems. In this talk I will discuss our novel concepts for all-optical switches based on semiconductor quantum wells which our modeling indicates are suitable for applications at these ultrahigh rates, even in single-channel operation. Moreover, these devices can be scaled down to tens to hundreds of microns. They may thus be suitable for hybrid spatial/time-division multiplexed systems far in excess of terabit/sec data rates.

Atomic Chain Electronics

Yamada, T.
NASA, USA

Due to the dramatic reduction in MOS size beyond 0.1 μm, there appear many unwanted effects. For example, the number of dopant atoms in the channel is not macroscopic and electrons may suffer significantly different scattering from device to device. This prohibits integration, but it is impossible to control

such dopant positions within atomic scale accuracy. One of the fundamental solutions is to create electronics with simple but atomically precise structures, which could be fabricated with recent atom manipulation technology. All the constituent atoms are placed as planned, and the device characteristics are deviation-free, which is mandatory for integration.

Atomic chain electronics [1] belongs to this category. Adatom chains are the component of devices, and are placed on an atomically regulated substrate surface without forming chemical bonding with substrate atoms. We can design the band structure and the resultant Fermi energy by manipulating the lattice constant d. Using the tight-binding theory with universal parameters, it has been predicted that Si chains are metallic and Mg chains are semiconducting, regardless of d [1]. For electronic applications, it is essential to establish a method to dope a semiconducting chain. If we replace some of the chain atoms with dopant atoms randomly, the electrons will see random potential along the chain and will be localized strongly in space (Anderson localization). However, if we replace periodically, although the electrons can spread over the chain, there will generally appear new bands and band gaps. In order to overcome this dilemma, we may place a dopant atom beside the chain at every N lattice periods (N>1). Group I atoms are shown to be donors and group VII atoms are shown to be acceptors. All of these predictions are based on the assumption that the chain atoms do not form chemical bonding with the substrate atoms and the substrate does not play a major role in deciding bands. This point will be examined, together with the possibility of adopting a scheme to allow chemical bonding for a maximum mechanical stability of the chains.

1. T. Yamada, J. Vac. Sci. Technol. B 15(4), 1019 (1997); ibid., A 15(3), 1280 (1997); T. Yamada, Y. Yamamoto, and W.A. Harrison, ibid., B 14(2), 1243 (1996).

Web-Based Computing

Richey, D.M., Finnerty, J.D., Singhal, K. and Tauke, J.D.
Lucent Technologies, USA

This paper describes a process for providing computational services to customers via the World Wide Web (WWW). The process involves users submitting job requests along with any necessary data through an HTML form accessible by a web-browser. Unlike typical internet applications which provide access to stored data in response to simple queries, this process provides users with advanced computational services for solving specific types of scientific and engineering problems. User-specified data is transferred to a computer server over the internet. The computer server processes job requests and informs users, via e-mail, once solutions are available. The users may access solution results using a web browser.

In this system, the user's web browser provides the interface for both input and output. Thus, multiple computational tools may be provided which all have the same look and feel to the user. This is particularly important for infrequently used applications. The computer software is not the responsibility of the user, as it is with the native running applications. The user does not have to obtain, install, or maintain the software. The computing power is not a function of the user's hardware, but rather the computer server. This lets the computing hardware (processor speed, system memory, mass storage) be matched to the computational task. The user does not have to buy expensive, but infrequently used, computational software, but may instead purchase services on an "as needed" basis. The users always have access to the latest version of the software.

This system provides several advantages for the software provider as well. Conventional software manufacture and distribution is eliminated. Requirements for multiple platform and operating environment support are also eliminated. Software testing is only required for one environment. In this way, testing is reduced by the number of different environments that would otherwise have to be supported. Support in general is greatly reduced, and field support is not required. Charging is directly related to usage, which greatly simplifies pricing. Time to market for enhancements is greatly reduced. Software can be optimized for one particular computing hardware configuration. This provides increased efficiency, lower cost, and higher value added for the customer. The entire sales and marketing process is simplified and reduced, resulting in large cost savings and higher value for the customer.

Session: H1-4 Room: CUB B1-5 **Time:** T9:30a-11:30a
Chair: *O. Awadelkarim (Penn State)*

Plasma-Etching-Induced Damage : Impact on Performance and Reliability of Submicron Field-Effect Transistors

Awadelkarim, O.O.
The Pennsylvania State University, USA

Three types of damage mechanisms in sub-half-micron metal-oxide-silicon field-effect transistors resulting from polycrystalline silicon (poly-Si) gate definition and metal interconnect plasma etch processes are reviewed in terms of their impact on transistor's performance and reliability. These mechanisms are : (1) inductive damage which arises from inductive coupling between interconnect circuitry and time-varying magnetic fields during plasma exposure; (2) damage induced by metal layout coupled with plasma nonuniformities and arising from electrical stress in the form of hot carrier injection or Fowler-

Nordheim tunneling at the gate oxide edge: and (3) plasma exposure and bombardment damage. These damage mechanisms are shown to be distinctly different from the well-known plasma charging damage which is dependent on poly-Si antenna ratio and which is healed by a 400 °C 30 minutes anneal in forming gas.

Current Ramp Testing for in-Process Screening and Monitoring of Electromigration

Cross, R.T., Ditali, A. and Hasnain, Z.
Micron Technology, Inc., USA

This paper presents a technique for evaluating and monitoring the effects of various processing steps on the electromigration susceptibility of single and multilevel thin film metalization at the wafer level. Through modification of the BEM technique[1], a ramp current stress test has been developed with sufficiently high throughput to enable its use as an in-line monitor as well as a screening tool for process development. The ramp current test is done by ramping a stress current on a metal test structure until an open condition occurs. The current to breakdown is recorded for a representative sample across a wafer or lot. From the breakdown data a mean current to breakdown (I_{50}) and standard deviation are obtained. Correlation between I_{50} and standard deviation and conventional constant current stressing at elevated temperatures have been obtained. Whereas the conventional electromigration test requires upwards of months to complete, the ramp current test is performed in less than 5 seconds per sample.

Examples of the utility of the ramp current test to develop a reliable double metal process will be presented. In this example it will be shown that ramp current stressing accurately predicts an optimal ILD thickness for a fixed via etch and metal deposition scheme. Conventional electromigration testing confirms the prediction of the ramp current test. In another example, we will show that the ramp current test is also viable as an in-line monitor of process deviations that would result in reduced metal reliability. In this case, narrow metal lines were processed in such a manner that voiding was present in the line prior to stressing. Two-point resistance measurements, as are typically performed at in-line parametric test, did not reveal a significant increase in overall line resistance. Careful and time consuming optical scans indicated the presence of voiding. On the other hand, the ramp current test also exposed the voids but in a much faster and more accurate electrical test.

C.C. Hong & D.L. Crook, "Breakdown Energy of Metal (BEM) – A New Technique for Monitoring Metallization Realibity at Wafer Level," Proc. IRPS, pp. 108-114, (1985).

Observation of Degradation Effects on MOSFETs from Interlayer Dielectric Processing

Trabzon, L. and Awadelkarim, O.O.
The Pennsylvania State University, USA

We report on the impact of plasma-enhanced chemical vapor deposition (PECVD) of fluorinated silicon oxide (FSO) and TEOS, high-density plasma (HDP) deposition of FSO, and spin-coating of low-k polymer as interlayer dielectrics (ILDs) on the characteristics and Fowler-Nordheim (FN) reliability of n-type metal-oxide-silicon field-effect transistors (MOSFETs). Transistor parameters were measured before and after FN stress. We found out that FSO deposition results on the highest degradation to the MOSFETs, whereas using the low-k polymer as an ILD yields the best performing and most reliable MOSFETs. We also examined the interaction between ILD growth and plasma charging during polycrystalline silicon gate-definition etch. For both types of FSO depositions we observed a reverse antenna correlation in that the larger the antenna the lesser the degradation incurred by the MOSFET.

An Atomistic Simulator for Thin Film Deposition in Three Dimensions

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Lawrence Livermore National Laboratory, USA
Gilmer, G.H.
Bell Laboratories, USA

As miniaturization of semiconductor devices continues, filling trenches/vias becomes increasingly difficult. A robust simulator can help interpreting experimental results and guiding further experiments. A large effort has been devoted to developing robust simulators (e.g., SPEEDIE, SAMPLE, EVOLVE, DEPICT, SIMBAD, etc.). A lot have been learned using these simulators.

However, as device size reaches deep submicron (0.25 to 0.10micron), width of the trenches/vias is on the order of hundreds of atomic layers. Atomistic processes dictate the deposition processes and must be treated at the corresponding level. Another important process, grain structure evolution, deserves better understanding in order to control film structure/texture.

Using a hierarchy of simulation methods (ab initio, molecular dynamics, Monte Carlo) and experimental results, we develop an atomistic simulator. The molecular dynamics is employed to obtain information on atomic movement at fine time (pico- to nano-seconds) and space scale (nanometers). The ab initio and experimental results serve to calibrate the molecular dynamics results. A three dimensional lattice Monte Carlo model has been developed to study long time (up to hours) and large scale (microns) processes. A site in the lattice can be occupied by an atom from direct deposition or diffusion. A site on single crystal

lattice is used to represent sites of all possible rotated lattices. A grain boundary is represented by high energy lattice sites, which are a result of carrying "mismatching bond". Mass transport along grain boundaries is simulated by two processes: local reorientation and single atomic jump facilitated by higher vacancy concentration, and their sum is matched with the molecular dynamics result. Microstructures, such as void and grain structure (nucleation, coarsening, and grain boundary grooving), of a thin film can be studied using this simulator.

Session: H1-5 Room: CUB B1-5 **Time:** T1:00p-3:00p
Chair: *P. Pedrow (WSU)*

Plasma Processing Of Electro-Active Polymers And Devices

Pedrow, P.D., Hoagland, R.G.Mahalingam, R. and Osman, M.A.
Washington State University, USA

Polymers have a long history of use as insulators to prevent conduction of electricity from one electrode to another. More recent research has investigated how polymers might be used as conductors of electricity and as "smart" material, which changes certain properties when activated by an electrical signal. Applications include control of electrostatic charge, batteries, drug delivery devices, optical switching, capacitors, optical displays, capacitors, microactuators, field-effect transistors, and light emitting diodes. Conventional electro-active polymers are formed from liquids or from neutral vapors. Our work will determine if plasma polymerized materials exhibit electroactive properties. Structures such as resistors, capacitors, field effect transistors, light emitting diodes and microactuators will be constructed and tested for electroactive properties. A pulsed plasma source facilitates production of the thin polymer films and includes doping of films and production of composite films. Film thickness will be in the range 5 to 500 nm. Present monomer capabilities include acetylene, ethylene, aniline and styrene. Parameters to be controlled and studied include electrical conductivity, electrical permittivity, electrostriction, film stress, film adhesion, and energy input per unit of monomer. This later parameter is expected to have an important influence on degree of cross-linking and concomitantly electroactive properties.

Short-Channel SOI MOSFETs Threshold Voltage Modeling with Induced Substrate Effects

Imam, M.A.
Motorola, USA and
Osman, M.A.
Washington State University, USA

A simple analytical threshold voltage model for short-channel fully depleted SOI MOSFETs has been derived. The model is based on the analytical solution of the two dimensional potential distribution in the silicon film (front silicon), which is taken as the sum of the long-channel solution to the Poisson's equation and the short-channel solution to the Laplace equation, and the solution of the Poisson's equation in the silicon substrate (back silicon). The proposed model accounts for the *traditionally ignored* [1-6] back gate substrate induced surface potential effects (SISP) at the buried oxide-substrate interface which contributed an additional 15-30% reduction in the threshold voltage. Conditions on the back gate supply voltage range are determined upon which the surface potential at the buried oxide-substrate interface is accumulated, depleted, or inverted.

In Fig. 1, the model predicted threshold voltage is plotted as a function of channel-length with and without the effects of SISP. Also shown are PISCES 2-D simulation results which agree well with the model predictions with SISP included. SISP importance is clear as it resulted in a threshold voltage reduction of 30 mV for the device simulated. In bulk silicon devices, 30 mV reduction will give about 5% reduction (assuming a technology with 0.6 V threshold voltage) which is not important and is generally considered as the wafer (or wafer-to-wafer) variation. In the SOI case, the threshold voltage is relatively small (0-0.2 V in many technologies) which causes 30 mV reduction to have a considerable reduction percentage (up to 30%) and therefore indicating the importance of SISP in the threshold voltage modeling. Because 30 mV variation is considerable in SOI technology, more tighter SOI processes are to fabricated with small variation windows for better process controllability.

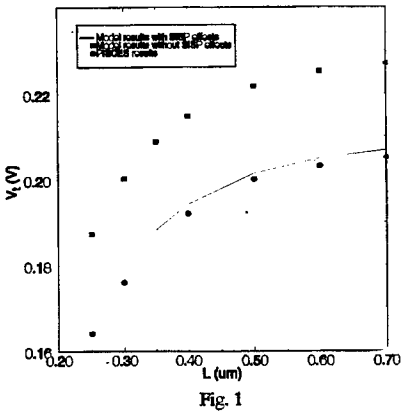


Fig. 1

[1] J.P. Colinge, Kluwer Academic Publishers, MA, 1991
[2] K.K. Young, IEEE Trans., ED-36, 1989
[3] S. Veeraraghavan, et al, IEEE Trans., ED-35, 1988
[4] J.C. Woo, et al, IEEE Trans., ED-37, 1990
[5] M. Imam, et al, Electron. Lett., 29, 1993
[6] S.R. Banna, et al, IEEE Trans., ED-42, 1995

Third Order Current Cancellation In HBTs

Wong, P.K. and Pejcinovic, B.
Portland State University, USA

A detailed understanding of third order current cancellation in HBTs is important in designing transistors and circuits with improved intermodulation distortion (IMD) performance. Considering the HBT's exponential nature, the linearity of actual devices is often better than expected. Possible explanations include current cancellation in the emitter-base junction, current cancellation at the base node, or the influence of emitter resistance. Using a simplified HBT model, we have derived analytical expressions that qualitatively and quantitatively describe 3rd order current cancellation.

The simplified HBT model sets the gain to $\alpha = 1$ and omits the emitter resistance R_{ee}. The equivalent circuit can then be separated into an R_bC_{be} part and a part containing only g_{be} and the current source. The nonlinear capacitance C_{be} develops the voltage that drives the current through the B-E conductance. The nonlinear conductance is defined via $i_g(t) = g_1v(t) + g_2v(t)^2 + g_3v(t)^3$ while the nonlinear charge in the capacitance is $q(t) = c_1v(t) + c_2v(t)^2 + c_3v(t)^3$. Fourth and higher order terms are neglected. The method of nonlinear currents is used to derive the analytical 3rd order expressions.

The nonlinear analysis produces an equation for $i_g(t)$ with eight different terms at the frequency $2\omega_1 - \omega_2$. From phasor plots of the $i_g(t)$ components, two types of cancellation mechanisms are apparent. The first is not current cancellation, but rather a cancellation between V_{be} voltages at $2\omega_1 - \omega_2$ across the nonlinear C_{be}. The second mechanism is true current cancellation due to phase differences within the E-B conductance. Harmonic balance simulations using H-P MDS were performed to verify the predictions from the analytical expressions. For more realistic cases in which $\alpha \neq 1$ or $R_{ee} \neq 0$, closed-form 3rd order expressions are difficult to derive, so only MDS results are presented for various gain, emitter resistance, and frequency parameter values.

The computer simulations and analytical equations for the simplified HBT model agree very well over a large frequency range. For $\alpha \approx 1$, there is still good agreement at higher frequencies. Adding emitter resistance improved the linearity of the circuit model by enhancing current cancellation. The equations and models developed enable us to examine the physical causes and offer interpretation of the measured data. Based on this knowledge we can then address the issue of design and optimization for minimum IMD.

Manganese Oxide Films for the Positive Electrode in the Li Secondary Batteries

Isai, M., Yamaguchi, K., Nakamura, T., and Fujiyasu, H.,
Shizuoka University, Japan and
Ito, Y.
Suzuki Motor Co., Japan

Manganese oxide films for lithium secondary batteries were prepared using a reactive evaporation method. Mn was evaporated by Hotwall epitaxy and deposited on a glass slide under oxygen atmosphere. The dependence of substrate temperature and oxygen flow rate on film quality was investigated. The MnO films with (200) preferred orientation were obtained at the substrate temperature lower than 350^{0}C. It was also found that the relative intensity of (200)/(111) was decreased with increasing the substrate temperature. The value of (200)/(111) was not varied with varying the flow rate of oxygen. The feasibility of varying the O2 valency in the Mn oxide films was investigated in the present paper.

Symposium H2
Mechanics and Sensing in Manufacturing Processes
Organizer
A.E. Bayoumi
North Carolina State University, USA

Session: H2-1 Room: CUB 214-16 **Time:** T3:30p-5:30p
Chairs: *J. W. Eischen (NCSU)*
C. D. Rahn (Clemson U.)

Automated Tailored Garment Manufacture: The Japanese National Project

Berkowitch, J.E.
National Textile Center, USA

A nine-year project supported by the Japanese Government and industry has established the feasibility of completely automating the manufacture of tailored garments, the most technically demanding class of apparel. The process called for having a bolt of fabric at one end and the finished garments ready for shipment at the other, without the intervention of human hands in between and without sacrifice of quality. Additionally effective manufacturing time was expected to ultimately be cut in half. The development broke ground in several areas which warranted over 200 patent actions. Advances in the handling of flexible materials deserve a special mention, particularly the introduction of mobile three-dimensional sewing heads mounted on multiaxis robot arms.

The project met most of its objectives by the time it concluded in 1990. A temporary semiworks facility produced women's tailored jackets of various sizes, made of woven and knit fabrics, each being either patterned or dyed in solid colors. Economics however have so far prevented commercialization of a complete line. The on-going migration offshore of Japan's manufacturing base and the recent turnaround in the general economy have made such a realization in the near-future even less likely. Instead, segments of the demonstrated technologies optimized for specific applications are gradually finding their way into the industry.

An introduction to the organization of the project and its technical challenges sets the stage for a 20-minute video presentation illustrating the fabrication of women" tailored jackets at the above facility. Major modules are described and shown performing fabric inspection, part cutting, presewing part preparation, two/three-dimensional sewing, and garment pressing. In summing up the teachings of this development, the conclusion points out the determinant role played by the advances in fabric mechanics fundamentals of the last two decades without which this sophisticated extension of robotics to flexible materials would have been impossible. In particular, tailorability, that is tailoring quality, a property expressed so far subjectively, has had to be programmed, hence for the first time defined quantitatively by means of basic fabric mechanical parameters measured in the laboratory under simulated end-use condition.

Quantitative specifications of the equipment demonstrated are addressed in a second video-of the same length of time-which can be passed in a separate informal session if warranted.

Engineering Analysis of Limp Material Properties Drives Design of Electromechanical Monitoring System

Clapp, T.G., and Titus, K.J.
North Carolina State University, USA

The design of any system requires a fundamental knowledge of the raw materials to be processed. This is especially true in the design of machines to handle and process limp materials such as film, fibers, and thin elastomer products. Traditional design rules and mechanical systems for processing rigid objects cannot be uniformly applied to successfully design robust processing systems. The machine design strategy should begin with a fundamental engineering knowledge of raw material property behavior under external conditions such as force, light, or heat. The mechanical designer can then incorporate this information in the design of a robust system. This paper describes the engineering design process that began with an analysis of denim fabric material properties. These properties include binding modulus, transverse and longitudinal compression characteristic, and surface properties. This analysis drove the design of an electromechanical system to evaluate proper construction of the joining (seaming) process in garment assembly. Design parameters such as contact area, applied force, and geometric considerations were optimized for the measurement of compressed seam thickness. A robust electromechanical system has been designed, constructed, and commercially-proven based on this design methodology.

Computer Simulation of Fabric Draping

Eischen, J.W. and Bigliani, R.
North Carolina State University, USA

Fabric drape and manipulation has only recently been simulated successfully because proper physical models and/or computational strategies have not been available. The automotive and aircraft industries (as well as many others) have adopted computer-aided-design/computer-aided-manufacturing approaches to streamline the design and manufacturing processes. Adopting these concepts to the textile and apparel industries is crucial for increasing competitiveness in those industries. This technology will allow increased

flexibility, higher quality, and fast response times. To fulfill these requirements, factories are considering increasing use of automated facilities in their conventional production lines. In the fabric assembly area, among the processes such as folding. For the future design of fabric products with variable material properties (weight, stiffness, etc.), a simulation capability is highly desirable. In this paper, a simulation capabilities that fulfill these requirements are described. Comparisons between geometrically exact finite element shell formulations and so-call "particle models" are made. Several examples of drape and manipulation problems of practical interest in the textile industry are shown.

Iterative Techniques for Fabric Position Control During Folding

Mast, S.O., Rahn, C.D. and Paul, F.W.
Clemson University, USA

Flexible automation allows apparel manufacturers to respond quickly to rapidly changing market conditions while minimizing skilled labor. Successful automation in the apparel industry has primarily been limited to fixed automation using special purpose, mass production machines. Flexible automation using general-purpose machines is difficult because the limp nature of the fabric complicates actuation and sensing, thus adding cost and complexity. A wide variety of materials need to be handled with diverse bending stiffnesses, weights, and frictional characteristics. Additionally, these characteristics vary from part to part and with temperature and humidity. Dependable flexible automation requires feedback to adapt to these variations. This paper develops and experimentally implements iterative algorithms for fabric folding with precise position control. A robot system folds the fabric, measures the resulting position using a vision system, and corrects the folding trajectory. The system adapts to changing fabric parameters, friction, and folding speed. Position errors of less than 1.2 mm are achieved within 6 folds for limp fabrics. Stiff fabrics require more complex control algorithms and additional folds to obtain similar position errors.

Session: H2-2 Room: CUB 214-16 **Time:** W9:30a-11:30a
Chairs: *Y. S. Lee (NCSU) &*
O. A. Abu Zeid (U. United Arab Emirates)

Geometric Modeling and Tool Placement Problems For Multi-Axis CNC Complex Surface Machining

Lee, Y-S.
North Carolina State University, USA

This paper presents the geometric modeling and algorithms to compute milling cutter placement and machined surface error analysis problems for 4- and 5-axis finished-surface machining. Different types of endmill cutters, such as torus-shaped (filleted) endmill, flat-endmill, and sphere-endmill, are used for multi-axis CNC machining. A generalized tool description with tool orientation variables for variant types of cutters is developed for multi-axis machining. Methods of finding an instantaneous cutting profile and the local surface geometry to analyze machined surface errors are discussed for cutter location generation. A method of deciding tool orientation to avoid rear tool collision using global geometry information is also presented.

The techniques presented in this paper can be used to eliminate errors of milling tool path generation in the area of simultaneous multi-axis CNC complex surface machining.

On the Mechanistic Modeling of Milling Cutting Forces: Hole Making Using an End-Mill Cutter

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Drilling is the most efficient machining process for making holes. However, with the rapid transition nowadays towards manufacturing automation and intelligent machining systems, hole making using milling cutters can be advantageous in many cases, when the vertical direction feeds are small, holes are shallow, and the hole making process is of short time duration. Less set-up and handling time, fewer tools to use, and simpler machine tool and fixture configurations can be achieved. Drilling and milling tools have similar geometrical features. The drilling tool is designed so as to utilize the bottom cutting edge for hole making, and the side cutting edge is rarely used. The milling cutter, on the other hand, is designed so as to utilize the side cutting edge for peripheral milling, and the bottom cutting edge is rarely used. In this study, a mechanistic model for cutting forces in hole making operation using an end-mill cutter is developed. The geometrical features of the bottom cutting edge of the end-mill cutter are considered and the total cutting forces are related to the process-dependent parameters: rake normal pressure, rake friction, and chip flow angle. In addition, experiments were carried out to investigate the variation of the process parameters along the cutting edge, which would be quite useful in tool design and automation.

Experimental Modeling of the Machining Characteristics Of EDMed AISI T1 High Speed Steel

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Electrodischarge machining (EDM) is a nonconventional manufacturing process used for precision machining of hardened steels, high strength and high temperature alloys used in the aerospace, automobile and tool and die industries. The process finds potential applications in areas such as manufacturing of intricate and complex designs and manufacturing parts with close dimensional control. The recent developments in EDM-related technology such as CNC EDM, automatic electrode changing, electrode orbiting and others have created a wide range of new applications for the EDM process. However, in spite of these technological advances, a highly skilled operator has to check periodically the progress of the machining and adjust the servohead. This has been reported to reduce the performance efficiency of the EDM process. In order to increase the process efficiency and help its integration into flexible manufacturing systems, it is necessary to explore ways of automating the process by introducing programmed controls which depend on both theoretical and experimental modeling of the EDM process. In this paper, mathematical models based on experimental measurements have been developed using Minitab computer program. These models correlate the metal removal rate, electrode wear and surface roughness of electrodischarge machined AISI T1 high speed steel with voltage pulse on and off times. Analysis of variance has been performed for the results obtained so as to study the significance of the effects of both on and off times and the adequacy of fit for the mathematical models. All experiments have been conducted using a transistorized pulse generator, copper electrodes, kerosene dielectric, side flushing, positive polarity and a current setting of 31.2 A. Constructed models have shown a strong influence for the pulse on time on the metal removal rate, electrode wear and surface roughness of the machined surfaces. On the other hand, the pulse off time has been observed to have comparatively little effects on the same machining characteristics.

A New Model for Chip Dynamics in Machining

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We present a new model for the dynamics of chip formation in machining. Our model differs from existing analytical models of metal cutting by including the local distribution of stresses applied by the cutting tool to the workpiece at the tool-material interface. Coupled with the transport of heat from this interface, this provides a mechanism for thermomechanical feedback in a nonlinear system, and leads to a model which is similar to models of chemical combustion processes. As the tool cutting speed increases, the strain rate in the material also increases, and a Poincare-Andronov-Hopf bifurcation occurs in the system, where steady-state behavior changes to oscillations in stress and temperature at the tool tip. These oscillations, which grow rapidly into relaxation oscillations, correspond to the formation of adiabatic shear bands in the chips. This exchange of stability from a steady state to elastic-thermoviscoplastic relaxation oscillations with increasing cutting speed provides an explanation for the change from continuous to segmented chip formation during the machining of hard materials, where it is often observed that the tendency towards chip segmentation increases with the cutting speed.

Mathematical Background of *CAM* System For Sculptured Part Surface Machining on Multi-Axis *NC* Machine Tool

Radzevich, S.P.
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The problem of efficient control of multi-axis machine tool while machining sculptured part surfaces is under consideration for a long period of time. In general this complicated engineering problem consists of mathematical description of the process of machining and of developing perfect software to efficient control of multi-axis machine tool in such manufacturing process.

To solve the geometrical and the kinematical part of the problem of effective machining of sculptured part surfaces on multi-axis machining tool the new so called *Differential Geometric Approach of Sculptured Part Surface Generating (DGASPSG)* has been developed [see: Радзевич С.П *Формообраз оание слонсных по ерхносмей на сманках с ЧПУ* - Киев: Виuа цкола (Radzevich, S.P., *Multi-Axis NC Machining of Sculptured Part Surfaces,* Vischa Shkola Publishing House Kiev, 1991, 192p. – In Russian)].

In *DGASPG* we use natural kind of representation of the sculptured surface P of the part to be machined and of the machining surface T of the cutting tool in machining operation, i.e., representation in terms of the first $\Phi_{1.P(T)}$ and of the second $\Phi_{2.P(T)}$ fundamental forms of the surfaces $P(T)$. Bonnet showed (1867) that the specification of the first and the second fundamental forms determines a unique surface if the Gauss equation (his *theorema egregium*) and the Codazzi-Mainardi equations of compatibility are satisfied, and that two surfaces that have identical first and second fundamental forms must be congruent.

Completed analytical description of the process of sculptured part surface *P* machining on multi-axis *NC* machine tool can be obtained only in a common to the both surfaces *P(T)* coordinate system. This caused the necessity of application of matrix method of coordinate system transformation which is widely used in *DGASPSG*.

To optimize the parameters of the process of multi-axis *NC* machining of sculptured part surfaces we have introduced (1983) a new class of functions – so called *functions of conformity* which are the geometrical analogues of productivity of machining operation. Efficient example of the functions of conformity is *an indicatrix of conformity* of the surfaces *P(T)*. Indicatrix of conformity of the surfaces *P(T)* is a plane curve of the fourth order which is located in a common to the surfaces *P(T)* tangent plane and which shows optimal direction of the surfaces *P(T)* relative motion. In *DGASPG* indicatrix of conformity yields to calculate the parameters of optimal toolpath, optimal parameters of the design of the cutting tool for sculptured part surfaces machining, to solve other geometrical and kinematical problems of multi-axis *NC* machining of sculptured part surfaces.

Session: H2-3 Room: CUB 214-16 **Time:** W1:00p-3:00p
Chairs: *A. E. Bayoumi (NCSU) & K. Awan (U. of Tech.)*

Feature Based CAD system for Axi-symmetrical Objects

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The most commonly used components in Mechanical Engineering are the axi-symmetrical objects (i.e. objects, which has symmetry around a central axis of rotation). These types of components are manufactured on the lathe machines by using turning operations. The lathe machines technology has improved in last few decades with the implementation of CNC (Computer Numerical Control) technology into the lathe machines. Now it is possible to automate design to manufacture process on these lathe machines by implementing CIM (Computer Integrated Manufacturing) concepts.

AutoCAD is wildly used as a Drafting package in the design industry. Usually a designer designs and draws an axis-symmetrical object by using a CAD (Computer Aided Design) package. This drawing is then passed on to the manufacturing engineer who generates the manufacturing information by using these drawings. In this work, a software system is developed which automates this process of design to manufacture and hence reduce the design to manufacture cycle time. The system extracts the axi-symmetrical information from the CAD drawing file (The file is in the DXF format). The extracted information is in the form of profile of axi-symmetric object. The program also checks whether the object is axi-symmetric or not. It also identifies different features (like turning, facing, grove, boring etc.) of the lathe operations. These features may be used to generate machine tool path for the manufacture of axi-symmetrical component. The software system is implemented on a Windows based PC platform by using C/C++ programming language.

A New CAE Interface In Virtual Shared Space

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We developed a new CAE interface to assist a collaborative design through the Internet. JavaTM and VRML were used to develop it. Through the interface users can easily access results that are analyzed by other users in remote site. The user can also communicate with other researchers or designers in the virtual shared space. The virtual shared space provides an environment for management of analysis results, in which the user can register comments about results and other user can read and examine them. Users in the world can conduct synchronous design process in the virtual shared space. The new interface was successfully utilized by international collaborative design project for micromechanisms.

Keywords: Lathe, Axi-symmetrical, CAD/CAM, feature recognition, CNC.

Breaking Mechanism of Chips in Intermittently Decelerated Feed Drilling

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This study involves a basic research to determine the optimum cutting condition with the main objective of revealing the breaking mechanism of the continuous cone-shaped helical chips produced during intermittently decelerated feed drilling. The friction torque due to chips flowing through the drill flute and the breaking torque of chips is determined experimentally and the breaking mechanism of chips in intermittently decelerated feed drilling was investigated. The following facts are ascertained from the obtained results. (1) Chips formed in intermittently decelerated feed drilling break at points where changes in chip thickness occur. (2) Breaking of chips occur when the resulting friction torque between the hole walls and chips is greater than the breaking torque of chips. (3) Chip breakage depends solely on the length of the fast feed section or the sum length of the fast feed and slow feed section and varies according to the intensity of the breaking force of chips.

Keywords: intermittently decelerated feed drilling, chip breaking mechanism, chip disposal resistance, breaking torque, aluminum alloys.

Gear Finishing Technology and Design of Gear Shaving Cutter

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Dnieprodzerzhinsk State Technical University, Ukraine, and
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Michigan State University, USA

A new approach of optimization of the parameters of diagonal gear shaving operation, i.e., optimization of the parameters of the gear shaving cutter design and the parameters of the relative motion of the gear to be machined and the gear shaving cutter has been studied.

The fundamental part of the problem under consideration is a derivation of the function for analytical description of the geometry of contact of the tooth surface P of the spur or of the helical gear to be machined and of the tooth surface T of the gear shaving cutter. For this purpose a new kind of characteristic curve so called *the indicatrix of conformity* of the surfaces P and T has been applied. This characteristic curve is a plane curve of the fourth order. It can be represented in a common tangent plane to the surfaces P and T. The minimal diameter of the indicatrix of conformity of the surfaces P and T coincides with the optimal direction of the gear to be machined and the gear shaving cutter relative motion in machining operation. This relative motion can be decomposed on rotations of the gear and the gear shaving cutter and on their relative translation motion in diagonal shaving operation.

To derive the equation of the indicatrix of conformity of the surfaces P and T vector representation of both of the surfaces has been used. Using matrixes of coordinate system transformation the equations of both of the surfaces P and T has been rewritten in a common coordinate system corresponding to the machine tool body. General representation of the indicatrix of conformity of the surfaces P and T (which has been earlier introduced by S.P. Radzevich) yields the equation of the same characteristic curve for the case under consideration.

The approach has been considered above gives a possibility to calculate optimal values of the parameters of the gear shaving cutter design and the parameters of the relative motion of the gear to be machined and the gear shaving cutter in machining operation.

Session: H2-4 **Room:** CUB 214-16 **Time:** W3:30p-6:00p
Chairs: *M. K. Khraisheh (King Fahd U) & M. Ketabchi (Tohoku U.)*

Recent Trends in Manufacturing Education

Bayoumi, A.E.
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Three Dimensional Analysis of Metal Flow In Extrusion of Non-Symmetrical Sections Based on Upper Bound Theorem

Ketabchi, M., Ikeda, K. and Murakami, T.
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Perhaps, the most important phenomenon in extrusion is metal flow because mechanical properties of extruded products depend on metal flow pattern during extrusion process. So analyzing and simulating of metal flow pattern which is quite comparable with experimental results is highly required. Also analyzing metal flow pattern may lead the development of an admissible velocity field by which an upper bound theory may develop. In this research extruding of U section from round billet has been investigated. Since this section is non-symmetrical, and because of some limitation in this section, mathematical analysis of this process is little bit difficult. This difficulty relates to making admissible velocity field. For this purpose the mathematical function of die surface from entrance to exit must be well defined. Since a flat face die has been used in this research, the mathematical development defining the die surface is the same as that of metal flow pattern. Effect of the shape of U section and its dimension on metal flow pattern also has been taken into account. For this purpose two kinds of U sections have been used and interestingly two kinds of metal flow pattern have been obtained. While in one die a round shape gradually changes to the die exit shape, in another die a specific intermediate section between entrance and exit section appeared.

Effects of Prebulging and Maximum Chamber Pressure in Hydromechanical Deep-drawing: a Finite Element Analysis

Zhang, S.H., Jensen, M.J., Kang, D.C. and Danckert, J.
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The hydromechanical deep drawing processes of aluminum cups and mild steel cups are analyzed by the explicit finite element code DYNA3D with various prebulging pressures, different maximum chamber pressures and different tool profile corners. The effects of prebulging deformation, maximum chamber pressures and tool profile corners on the final product

quality are discussed. The numerical results are compared with those obtained in experiments.

Relationship Between Joint Performance and Heat Input in Friction Welding

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Osaka Prefecture University, Japan
Kurozawa, T.
Setunan University, Japan, and
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Keio University, Japan

In this paper, friction welding of low carbon steel (0.16 %C) was carried out under the various welded conditions. During the welding process the friction speed and the friction torque were detected and recorded, and heat input was calculated using these factors in order to examine the relationship between heat input and joint performance. And, the effect of heat input on the joint performance such as tensile strength, bending strength, torsion strength, impact strength, hardness and microstructure at the welded interface was discussed.

Growth And Distortion Of Parts Due To Application Of Fasteners

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A large assembled part in an aerospace structure may have several hundreds to thousands of fasteners. Interference-fit fasteners and rivets produce locally compressive plastic strains and tend to improve fatigue strength of the work material. However, they also introduce unwanted distortion and growth of parts which may cause certain dimensions to exceed their tolerance limits. When fixtures are employed to prevent growth, then the application of fasteners introduce stresses in parts that can lead to premature failures of work material or fasteners. This paper employs both analytical elastic-plastic analysis as well as finite element analysis to predict growth and distortion of typical structural members due to interference-fit fasteners. Growth and distortion results are expressed as functions of both geometrical and material parameters of fasteners and work materials, i.e. diameter and interference of bolts, the yield strengths, and the geometrical shape and size of the work material. Analytical and finite element results are correlated with experimental results.

On Prediction of Fracture in Metal Forming Operations

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Fracture on the outside or inside of the workpiece has considerable influence on the success and economy of metal forming operations. It is well known that in ductile metals the hydrostatic component of stress and the equivalent plastic strain are the most important parameters in fracture analysis. In engineering practice the upper bound method is usually applied for the modeling of metal forming operations. However, using this method one cannot determine the hydrostatic stress. Moreover, kinematically admissible velocity fields usually involve velocity discontinuity surfaces. These surfaces may give a significant contribution to the fracture process since the equivalent plastic strain undergoes a jump across such surfaces (Even though such surfaces are seldom seen experimentally, they are very helpful for theoretical analyses). In order to account for this contribution and to determine the hydrostatic component of stress we combine Hill's general method of analysis for metal working operations and a workability diagram for bulk metal forming operations in terms of the triviality level and the plastic work. Using Hill's method allows us to find the hydrostatic component of stress. Using the plastic work instead of the equivalent plastic strain (the latter are usually used in definition of workability diagrams for bulk metal forming operations) allows us to take velocity discontinuity surfaces into account in fracture analysis in a natural manner, since the evolution equation for the plastic work can be transformed into divergence form. Note that if a material obeys von Mises yield criterion and a velocity field is continuous then the results obtained with the use of the equivalent plastic strain and the plastic work are the same. A procedure which allows one to determine the workability diagram in terms of the plastic work by using the known diagram in terms of the equivalent plastic strain is proposed. Moreover, a simple approach to find points of the workability diagram is developed. The approach is applicable if fracture occurs at a free surface and is based on experimental data and an analytical solution for the hydrostatic component of stress at the free surface. The analytical solution is obtained at large strains such that elastic portions of strain are negligible. Some of plastic components of strain should be determined experimentally.

The approximate approach proposed for fracture analysis of metal forming operations can be very effective for two dimensional and three dimensional steady processes by adopting different material models, in particular those for which other approximate methods are not applicable and numerical methods require many time steps.

The approach proposed to find the shape of workability diagrams is applied by using published experimental data for upsetting with profiling dies. It is shown that the approach predicts the shape of workability diagram in very good agreement with other methods, but requires less experimental work.

A numerical example, extrusion (drawing) of round rods, which combines ideas of both the approaches is given. In particular, the influence of die shape on the fracture process is discussed.

Symposium I1
Biomechanics and Biomathematics
Organizers
K. Campbell
Washington State University, USA
&
C. Martin
Texas Tech University, USA

Session: I1-1 **Room:** CUB 214-16 **Time:** T9:30a-11:30a
Chair: *C. Martin (Texas Tech) & K. Campbell (WSU)*

Some Modeling Issues in Hill-Based Systems

Schovanec, L.
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Phenomenological Hill-type models are extensively utilized by bioengineers and movement scientists investigations of multiple muscle systems. Roughly stated, these models consist of an active contractile element in parallel and in series with passive components. This paper explores some modeling issues in musculotendon dynamics and their significance in applications to gait and ocular movement. In particular, choices of internal states for the musculotendon actuator, tension-length and force-velocity relationships for the active contractile element, muscle mass, and the modulation of system components by activation are explored. The consequences of these assumptions are related to system dimension, controllability and computability. Specific implications of these modeling assumptions are illustrated in simulations of the head-eye system an din a direct dynamics analysis of gait.

A Direct Approach Utilizing Musculoskeletal Dynamics and Neuromuscular Control to Determine Stress Development in Bone

DeWoody, Y. and Schovanec, L.
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The role of forces produced by the musculotendon units in the stress development of the femur during gait has not been fully analyzed. It is well known that the musculotendons act as actuators producing the joint torques which drive the body. Although the joint torques required to perform certain motor task can be recovered through a kinematic analysis, it remains a difficult problem to recover the actual forces produced by each muscle that resulted in these torques. As a consequence, few studies have focused on the role of individual muscles in the development of stress in the bone.

This study takes a control theoretic approach to the problem. A 7 link, 8 DOF model of the body is controlled by various muscle groups on each leg to simulate gait. The simulations incorporate Hill-type models of muscles with activation and contraction dynamics controlled through neural inputs. This direct approach allows one to know the exact muscle forces exerted by each musculotendon through out the gait cycle as well the joint torques and reaction forces at the ankle and knee. Interpreting the muscle forces as tractions on the femur, finite element techniques are then utilized in determining the stress fields in the bone. Thus the role of individual muscle groups in the stress development of the femur gait can be analyzed.

Comparison Among Putative Myofilament Cooperative Mechanisms Regulating Cardiac Contraction and Relaxation

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Steady-state force generation by cardiac muscle exhibits a much more cooperative response to varying Ca^{2+} levels than can be predicted by the single regulatory site that binds Ca^{2+}. Several cooperative mechanisms have been suggested, and all of these can predict the observed, highly cooperative steady-state F-Ca relationship. Hence, such steady-state analysis is unable to distinguish clearly between different models of cooperativity. This study attempts to resolve the potential contribution of alternative cooperative mechanisms by testing model responses to a dynamic stimulus, not just a steady-state one. The dynamic stimulus simulated the natural rise and fall $[Ca^{2+}]$ that initiates a cardiac contraction-relaxation cycle.

Five models of cardiac myofilaments were structured around a functional regulatory unit of troponin., tropomyosin, and actin. The models contrasted with one another by combining different subsets of the three putative cooperative mechanisms (described below). They dynamic time course of isometric force generated by each model at various sarcomere lengths was compared to similar experimental data from the literature. By correlating model responses to the underlying cooperative mechanisms, the following conclusions were drawn:

Cooperative Mechanism 1 holds that crossbridge attachment increases the affinity with which troponin binds Ca^{2+}. In the models, Mechanism 1 can produce steep force-Ca^{2+} relations, but apparent cooperativity is highest at mid-level $[Ca^{2+}]$. During twitches, Mechanism 1 has the effect of increasing the time required to reach maximum force as the magnitude of force increases: this effect is not seen experimentally. In fact, only modest amounts of such cooperative feedback can be added before the dynamic behavior becomes inconsistent with experimental results.

Cooperative Mechanism 2 holds that the binding of a crossbridge increases the rate of formation of neighboring crossbridges, and that multiple crossbridges can maintain activation of the thin

filament in the absence of Ca^{2+}. Only Mechanism 2 can produce variable prolongation of relaxation dependent upon peak force development, but this mechanism cannot produce steep steady-state F-Ca relations.

Cooperativity Mechanism 3 simulates end-to-end interactions between adjacent troponin/tropomyosin units. This mechanism can produce steep F-Ca relations with appropriate sarcomere-length-dependent changes in Ca^{2+} sensitivity. With the assumption that tropomyosin shifting is faster than crossbridge cycling. Mechanism 3 produces twitches where the latency to peak is independent of the magnitude of peak force, as seen experimentally.

In summary, dynamic analysis suggests that both Mechanisms 2 and 3 must be significant in cardiac muscle, while Mechanism 1 can exert only a small influence.

Analysis of in Vitro Sliding Velocities Produced by Mixtures of Different Types of Myosin

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During the past few years, there has been an explosion in the number of identified myosin types. The vast majority are from cytosolic motile systems in which there is no large-scale, organized array of actin and myosin filaments. Thus the classical techniques developed to study muscle fiber mechanics are inapplicable. One technique that has proven to be extremely valuable is the in vitro, gliding assay. In this assay, the movement of fluorescently labeled actin filaments over a surface coated with myosin molecules is observed by video microscopy. The viscous drag on a sliding actin filament is significantly less than the mechanical force produced by the myosin cross-bridges. Thus the filaments are sliding at their maximal velocities. The source of actin has very little effect on sliding velocity. A wide range of sliding velocities have been observed for different myosin types.

In order to better understand the mechanism by which myosin produces force for biologically useful movement, we studied the in vitro sliding velocities of actin filaments generated by pairwise mixings of different types of actively cycling myosins. In isolation, the myosins translated actin filaments at differing velocities. We found that the observed sliding velocity of a mixture of myosin types was highly nonlinear with respect to the proportion of the more slowly translating myosin type. Only a very small proportion of a more slowly translating myosin would significantly inhibit the sliding velocity generated by a myosin type that translated filaments rapidly. In other experiments, noncycling, unphosphorylated smooth and nonmuscle myosins were mixed with actively translating myosin types. By themselves in in vitro assays, these myosin types translate actin filaments slowly, if at all. Sliding velocity of the rapidly translating myosin type was again inhibited. However, now a very large proportion of the noncycling myosin was required to significantly reduce the sliding velocity of the mixture.

In order to better understand these seemingly contradictory experimental observations (strong inhibition vs. weak inhibition of sliding velocity), the experimental data were analyzed using computer simulation of a multi-state crossbridge model based on the original working crossbridge model of A.F. Huxley (Prog. Biophys. Biophys. Chem 7, 258, 1957). The new model takes into account the experimentally established biochemical and biomechanical differences between actively cycling and noncycling crossbridges. In this context, the model suggests that the two distinct modes of inhibition are not contradictory. They are, in fact, precisely the behavior to be expected from current models of the actomyosin interaction.

Differential Equation for Crossbridge Distortion in Muscle Models

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Muscle force, $F(t)$, resulting from parallel, force-generating crossbridges, XB, undergoing cyclic transitions between force-generating, *fg*, and non-force-generating states may be given by $F(t) = kN_{fg}(t)X(t)$ where k is the stiffness of a single XB, $N_{fg}(t)$ is the number of XBs in the *fg* state, and $X(t)$ is the average distortion among the *fg* XBs. Dynamic changes in $F(t)$ resulting from changes in muscle length, $L(t)$, must take into account the dynamic length-induced changes in both $N_{fg}(t)$ and $X(t)$. Differential equations describing dynamic changes in $N_{fg}(t)$ are easily derived from the kinetic scheme adopted for the XB state transitions. For instance, kinetic steps leading from a precursor state, N_{-1}, into and away from the *fg* state may be represented $N_{-1} \xrightarrow{h} N_{fg} \xrightarrow{g}$ with a describing differential equation

$$dN_{fg}(t)/dt = hN_{-1} - gN_{fg} \qquad \text{(EQ 1).}$$

The differential equation describing the dynamic changes in $X(t)$ are not so obvious. The objective here is to provide such a differential equation.

The differential equations for $X(t)$ is derived by considering the summed distortion among all *fg* XBs as given by

$$Z(t) = N_{fg}(t)\,X(t) \qquad \text{(EQ 2).}$$

During isometric conditions, distortion is imposed by the powerstroke leading into the *fg* state which imparts an isometric distortion $X(t) = X_0$. Changes in $L(t)$ over a time interval Δt, causes changes in the summed distortion, $Z(t + \Delta t)$, according to

$Z(t + \Delta t) = Z(t)$ + *[added distortion among fg XBs due to change in length over* Δt*]* + *[added*

distortion due to formation of new XBs with X_0 distortion over Δt)] - [lost distortion due to detachment of distorted XBs with X(t) distortion over Δt)]

Substituting and taking the limit as $\Delta t \rightarrow 0$ yields,

$$dZ(t)/dt = N_{fg}(t)[dL(t)/dt] + [h\,N_{-1}(t)][X_0] - g\,N_f(t)X(t) \quad \text{(EQ 3)}$$

Differentiating (EQ 2) gives

$$dZ(t)/dt = [N_{fg}(t)/dt]X(t) + N_{fg}(t)\,dX(t)/dt \quad \text{(EQ 4)}$$

Equating (EQ 3) and (EQ 4), making appropriate substitutions for $dN_{fg}(t)/dt$ from (EQ 1), and solving for $dX(t)/dt$ gives the desired differential equation for average distortion among a population of parallel XBs

$$dX(t)/dt = -h\frac{N_{-1}(t)}{N_{fg}(t)}[X(t) - X_0] + dL(t)/dt \quad \text{(EQ 5)}$$

Thus, in response to a change in $L(t)$, the dynamics of $F(t)$ will include the dynamics of $N_{fg}(t)$ as given by EQ 1 and the dynamics of $X(t)$ as given by EQ 5.

Session: I1-2 **Room:** CUB 214-16 **Time:** T1:00p-3:00p
Chair: *K. Campbell (WSU)*

Thermoregulatory Models and Human Responses to the Environment

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Mathematical modeling of thermal responses allows testing of wide performance limitations in individuals exposed to environmental extremes. Use of models is therefore especially important when experimental settings with human subjects are restricted to finite thermal limits necessary to protect the individual. In essence, the ideal mathematical model of thermal strain should incorporate all essential variables active in thermoregulation. Although almost an insolvable task, a great many worthwhile models do a reliable job describing the heat balance equation. Models describing steady-state responses apply best when quasi-heat balance exists. Models are quite useful in a first approach prediction of physiological effector response (sweating rate, skin blood flow, etc.), particularly when a given metabolic activity stays constant over the time of the given exposure. A regulating system is usually described in two distinct ways: in terms of a passive or controlled system and an informational or controlling system. In physiological terms, the controlled system in human thermoregulation is considered as the body with its inclusive anatomical features, heat capacities, and energy fluxes from various tissues: core, muscle, adipose, and skin sites. The controlling system includes the complete central nervous system transmitting information in a network manner. Early forerunners of rational thermal models employ elements of heat exchange that predict physiologic response and incorporate extensive descriptions of the passive system in terms of a steady-state bio-heat equation. Other models describe open-loop systems without a full description of control or regulatory action. Such models have been established on a scanty experimental data base and offer closed-loop characterizations of the thermoregulatory system which include a rudimentary feedback control formulation of internal body temperature. In our Institute, a significant data base has been collected using human experimental studies and wide clothing systems from which predictive modeling equations can be developed for individuals working in various environments. This paper encompasses approaches conventionally used in both rational and operational models and presents a comparison between measured and predicted core temperature responses during exercise and environmental exposure. Test cases using several thermal models will be compared to show simulation techniques operable during cold stress and heat strain in athletic, industrial, and military settings. Future concepts and problems will be discussed involved in simulation schemes and reliability testing of model operations required in mimicking body temperature shifts, thermoeffector responses and circulatory changes in humans in extreme environments.

Multisystem Modeling: Pharmacologic and Neural Effects in Cardiovascular Models

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Mathematical simulation was a major motivating force for development of computers, and physiological simulations have been employed in physiological and medical curricula for almost thirty years. Still, computer simulations have met with mixed success, because most have been narrowly focused on individual topics and have not proven highly portable outside their own institutions. In order to develop mathematical physiology simulation of broader utility, we have addressed the problem of coordinating multiple simultaneous interactive models. This report discusses our simulation architecture and its application in coordinating pharmacokinetic, pharmacodynamic and cardiovascular mechanical models within a large scale model of human physiology.

Our models are contained in a program called SimBioSys, which stands for simulation of biological systems. This program, written in C++, has a cooperative time sharing system at is a core, and provides time slices to individual models. Each model consists of a set of computer instructions able to calculate outputs for a specified time. Some models use sets of differential equations, some invert systems

of equations, some elaborate stochastic processes, and others merely calculate algebraic expressions subject to elementary logical constraints. In each case, the computational machinery of the model is governed by the applicable physics and biology of the system being described. An object oriented program design enables an elegant and efficient matching of computational cycles to the needs of the physical models.

In this report, we will explain the application of the SimBioSys architecture to the problem of how neural and drug effects act as controls on a real time mechanical model of the cardiovascular system. Neural effects are calculated by second order differential equations describing sympathetic and parasympathetic tones. Drug kinetics are handled using kinetic models for absorption and elimination by various routes. A uniform acceleration factor is available to provide faster absorption and elimination, to permit the correct steady state to be achieved at a uniformly accelerated time for easier use in teaching. Drug receptor binding affinities are described for both agonistic and antagonistic binding. Drug models are instantiated at run time, so differential equations need be solved only for the subset of drugs actually used in a given simulation. Receptor occupancy information is passed to the cardiovascular models, providing real time access to effects of drugs and drug interactions on mechanical properties of cardiac mechanics, cardiac excitation, and arterial and venous properties.

The Mechanics of Undulatory Swimming: Virtual and Robotic Leeches

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Swimming with whole body undulations involves a mechanical interaction between an organism's tissues and its fluid surroundings. Unfortunately, we do not fully understand the form of this interaction, nor do we understand how variation in an organism's morphology and physiology may affect this interaction. It is readily apparent that the internal and external components of the swimming system are tightly coupled, and that the coupling plays a major role in determining the swimming behavior exhibited by whole body undulators. However, it is the coupled nature of the internal and external mechanics that makes the problem so challenging. Studied in isolation, the internal and external mechanical components of the swimming system may not be representative of their *in situ* behavior. To address this issue, as well as the form of the coupling and its sensitivity to the organism's morphology and physiology, we are taking a number of approaches. One, the 'virtual leech', is a mathematical model of a flexible body constructed from elements that have the mechanical properties of both active and passive biological elements that have the mechanical properties of both active and passive biological materials. The model is coupled to a simplistic representation of a fluid, however the approach explicitly accounts for the internal and external mechanics, as well as their interactions. Other approaches are essentially refinements on the above model: an immersed boundary method representation of a soft-bodied organism coupled to a Navier-Stokes fluid solver, and a mechanical undulator with prescribed morphology, kinematics and swimming speed with which we can measure the fluid-body interactions as a function of body form and swimming kinematics.

The Smoker at Great Depths: Seeking a Unification of Pathophysiology, Mechanics, and Fluid Dynamics

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On dives to simulated depths of 300 meters or more, respiratory resistance (R) increases with gas density ($\dot{\rho}$) in some divers at twice the rate of others, with elevated R's being associated with significant smoking histories. This phenomenon has been revealed by two independent techniques: transient flow interruption and the method of forced oscillation. This observation is puzzling because the flow resistance of smokers is generally not elevated at 1 atm abs; for fluid dynamic reasons resistance measurements are believed insensitive to the changes in small airways of asymptomatic smokers. This paper shows how equations of motion for a respiratory system with serial inhomogeneity can explain this effect of diving on smokers.

We used a previously published model of the respiratory system divided into central (c) and peripheral (p) airways with serially aligned resistance and inertance (L). Central resistance and inertance increased in proportion in $\dot{\rho}^{0.5}$. Cs and Crs was airway wall and respiratory system compliance, respectively. Smokers (S) had normal central airway resistance, but elevated peripheral resistance compared to nonsmokers (NS). The equations of motion for the model were found from the network impedance equations for a 2 rung ladder network. We then solved for the real (Zr) and imaginary (Zi) components of the input impedance spectra over the frequency range of 0 to 200 Hz, as in the forced oscillation method of measuring respiratory resistance. Resistance (R) was taken as the real component of impedance at resonance (Zi=0). R was also assessed at low frequency (0.5 Hz) to mimic the interrupter measurements.

At 1 atm, resonant frequency was much higher in the S condition than in the NS condition. In spite of this, R in smokers and nonsmokers was similar at 1 atm. In the NS condition at all depths, and the S

condition at 1 atm, the frequency of resonance and the minimum impedance magnitude coincided, but not in the S condition at depth. This uncoupling was associated with an elevation of R. R rose faster with ⚲ in the modeled smokers than in the nonsmokers. Fluid dynamic arguments do not explain these results because flow in the small peripheral airways, where smoking induced damage is first manifest, is believed to be fully laminar and therefore density independent. Computational fluid dynamic analyses based on pathologically altered small airways may eventually unify these observations.

Cardiovascular Model For Gravitational And Accelerative Stress

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Accelerative and gravitational forces (G-force) on the cardiovascular system cause a redistribution of blood volume and flow. To counter these effects, external pressure suits are widely used. However, design of these devices including body coverage, pattern and magnitude of suit pressurization, and coordination of suit pressurization with other corrective actions (posture adjustments, straining maneuvers, and positive pressure breathing) have largely been conducted by trial and error methods. This work was to develop a computer model of the human cardiovascular system as an aid in the design of external pressure suits for protection against unusual G-forces.

Although many cardiovascular models have been developed, none were perfectly suited for application to this problem. Thus, a cardiovascular model was constructed from the ground up. Blood vessels were represented as a branching arrangement of spatially lumped vascular segments, each segment with its own pressure-flow-volume relationship. Lumping and anatomical representation of the arterial and venous systems largely followed the pattern of Westerhoff . The volume capacitance of the smallest venous vessels was represented in the microcirculatory element connecting terminal arteries and veins. Changes in G-forces affected the hydrodynamic pressure profile in each vessel segment according to the segment's orientation with respect to the G-force. Unlike many previous cardiovascular models, special attention was given to realistically representing the nonlinear pressure-volume characteristics of each lumped segment. This was essential because blood volume redistribution during G-force is largely determined by these nonlinear characteristics including blood vessel closing and re-opening. The heart and pulmonary circulation were represented by two time-varying elastance-resistance pumps connected in-series with an intervening circulation. Model validation consisted of reproducing normal human hemodynamic values of central-venous pressure, arterial pressure, and cardiac output and normal regional blood flow distribution. Further validation consisted of reproducing normal left ventricular pressure-volume loops. When simulated G-forces were applied, the model responded according to expectation with predicted cerebral blood flow changes that depended strongly on the assigned posture. Dangerous decreases in cerebral blood flow were effectively prevented by simulated suit pressurization for accelerative stresses < 9 Gs.

Poster Session P1
Monday, September 28th, 1998
CUB Ballroom
All Day Event

Analytical Determination Of Cyclic Hydrostatic Stress-Strain Relations For A Composite Sphere With A Soft Inclusion And A Hard Bilinear, Isotropically Hardening Matrix

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This paper deals with the analytical determination of cyclic hydrostatic stress-strain relations for an inclusion-matrix concentric sphere. Both phases are taken to be elastically isotropic, and the inclusion is taken as elastically softer than the matrix. The matrix is taken to be bilinear and isotropic hardening is assumed. Yielding is assumed to occur in the matrix by the vonMises' criterion. Using Hill's(1950) approach as a starting point, the exact solution is first determined for the first five sequences of loading(i.e. alternate tensile and compressive loadings). Based on the developed equations for the first five sequences and an inductive approach, the analytical relation for the overall hydrostatic stress and strain for the N^{th} loading sequence is *suggested.* For the convenience of implementation, the resulting equations are given separately for stress and strain control. With the developed equations, the Bauschinger effect for the composite sphere is studied. Interestingly, it is seen that irrespective of the inclusion volume fraction , the relative stiffness of the soft inclusion/hard matrix or the work-hardening nature of the matrix, the composite response is initially governed by isotropic hardening, whereas an asymptotic response is approached where both kinematic and isotropic mechanisms play equally important roles. Such an evolution in the composite response is attributed to the evolution in internal stresses of the composite sphere.

Air Flow And Exhaust Dilution Rates From Johnson Hall Wind Tunnel Study

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Recently the personnel of Johnson Hall at Washington State University have experienced air quality problems, which might be caused by the re-entry of hazardous and odorous gases into the building through the air intake vents, and open windows. Atmospheric tracer gas experiments and boundary layer wind tunnel test were used to investigate the flow patterns and exhaust gas dilution rates for Johnson Hall and also the impact of exhaust gases from surrounding buildings. Several field experiments were conducted at Johnson Hall at prevailing wind conditions using Sulfur Hexafluoride (SF_6) as a tracer gas. Fume hoods were chosen as tracer gas release sites, because laboratories were thought to be the source of the toxic gases. Gas samples were taken at locations in and surrounding the building. The concentration results provided air flow patterns and dilution rates in and around Johnson Hall. The wind tunnel experiments were desired because the wind direction, wind velocity and stack were controllable in the wind tunnel. Flow visualization and SF_6 tracer studies were performed on a 300:1 scale model of Johnson Hall and surrounding buildings in a 3' x 3' blowing type wind tunnel. The roughness of the floor at the boundary layer section was adjusted to give a wind velocity profile with Z_o scaled at 300:1 to the field conditions. The experiments involved flow visualization which uses smoke to determine recirculation zones and SF_6 tracer technique which quantify the dilution factors at various locations on the model. The effect of stack height was also investigated. Experimental results about the flow pattern, recirculation zones, and exhaust gas dilution rates were analyzed to make the recommendations for possible solutions to minimize the re-entry of exhaust gases.

Different Methods to Determine the Surface Areas of Polar Molecules Absorbed on Solid Surfaces

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In a previous study, we proposed various models giving the molecular areas of n-alkanes and polar molecules: geometrical model, cylindrical molecular model, liquid density model, BET method and Kiselev result. In this paper, we used Redlich-Kwong equation transposed from three-dimensional space to two-dimensional space to calculate the areas of organic molecules. Two experimental methods were used to confirm the theoretical results: the inverse gas chromatography and the dynamic contact angle technique.

A New Method to Calculate the Surface Potential of an Air Bubble Moving Along an Inclined Surface

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The study of gas bubbles in general and air bubbles more particularly, are of vital importance in the chemical and mineral process industries. Air bubbles were widely used in microbiological processes in order to provide the necessary oxygen to the dispersed microorganism. By a complete analysis of the interaction forces between an air bubble and inclined surface in aqueous medium and taking into consideration the following forces:

- the electrokinetic lift force
- the buoyancy force
- the drag force
- the London-Van der Waals force

and the electrical double layer repulsion force we were able to find a relationship between the surface potential of the bubble and the other parameters of the problem, like the velocity of the air bubble, the zeta potential of the inclined solid surface, the reciprocal Debye-Huckel lengths of the electrical double layers, the electrolyte concentration, the permittivity of the medium and the separation distance between the spherical bubble and the surface. All these parameters can be experimentally measured.

This analysis allowed to obtain the surface potential of the air bubble by using the fixed point theorem.

Modeling of Dynamic Failure in a Wide Range of Temperature and Pressure

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In most of existing criteria for dynamic failure, effects of temperature and pressure are ignored. In a few recent contributions, attempts to include initial temperature effects have been proposed. However, pressure effects are still lacking in all existing criteria. The aim of the present work is to model the effects of both pressure and temperature on dynamic failure. We propose a unified approach that we have implemented within several dynamic failure criteria to simulate spallation at different initial temperatures and in a wide range of pressure.

We select some of existing failure criteria and apply them to simulate spallation in planar impact test. Results from this approach are discussed and compared with results without temperature and pressure effects.

Time-Dependent Subloading Surface Model For Soils

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The time-dependent subloading surface model proposed by the author (Hashiguchi, 1998) is applied to soils, which describes also the isotropic (volumetric and deviatoric) hardening and the anisotropic (rotational) hardening. Its adequacy is verified by comparing with some experimental results for undrained triaxial compression with various strain rates and stress relaxation.

A Parametric Study Of Void Growth In Superplastic Deformation

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Substantial void growth in metals constitutes a problem in many industrial operations that utilizes superplastic deformation. This is because of the likelihood of material failure due to such growth, eventually. Hence, there is a need to study void growth mechanisms in an effort to understand the parameters governing it. In this work, numerical and experimental studies of void growth, and the parameters that affect it, in a superplastically deforming (SPD) metal have been performed. In the numerical studies, a 1×2 sized thin plate (i.e. plane stress conditions) of a viscoplastic material with pre-existing holes has been subjected to a constant extension rate. The stress-strain solutions were obtained using the finite-element method. The experimental studies were performed under similar conditions to the numerical ones and provided for qualitative comparison. The parameters affecting void growth in SPD are: m (the strain-rate sensitivity), hole size (i.e. diameter) and the number of existing holes. The results showed that increased m values produced strengthening and decreased the rate of void growth. In addition, larger initial void size (or, equivalently, a larger initial void fraction) had the effect of weakening the specimen through causing accelerated void growth. Finally, multiple holes had the effect of increasing the metal ductility by reducing the extent of necking and its onset. This was realized through diffusing the plastic deformation at the different hole sites and reducing the stress concentration. The numerical results were in good qualitative agreement with the experiment and suggested the need to refine existing phenomenological void growth models to include the dependence on the void fraction.

Study Of Forced Convection Boiling In Microgravity

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Forced-convection subcooled nucleate boiling has been recognized as one of the most efficient terrestrial heat transfer mechanisms. Forced-flow boiling in microgravity has also received some attention. Researchers have been trying to determine the effects of loss of gravity on the forced-flow boiling heat transfer and how to maintain the high efficiency in space.

The present work provides experimental data and flow visualization results for forced-convection boiling over a gold-film flat surface heater in microgravity. Specifically, nucleate boiling curves, heater surface temperatures, heat transfer coefficient, and heat fluxes for various forced-flow conditions are presented. A flow boiling regime map developed based on

photographic results of bubble sizes and patterns are introduced to facilitate physical understanding.

In order to study the details of a single vapor bubble, a thin gold film semi-transparent heater was designed and used to generate single bubble. Bubble generation, growth, and departure in microgravity with different flow rate were observed by CCD camera. It was found that the bubble diameter seems to be proportional to the parameter of ($Re^{-1/3}t^{*1/3}$). It was observed that the high flow rate would offset the microgravity effects. As a result, the bubble generation frequency, Weber number, and bubble shape tend to be similar with that in normal gravity.

Critical heat flux (CHF) and the transition from nucleate boiling to film boiling in flow field is another important aspect in the present research. Predicting the CHF is significant in heat transfer design as film boiling often leads to catastrophic increases in the heater temperature. In particular, visualization of bubble generation on a platinum wire heater will be provided by CCD camera. Also, the corresponding heat flux and surface temperature relationship will be studied.

Effects of Self-Heating on Gate Transconductance (g_m) of Silicon-On-Insulator MOSFETS

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Self heating is pronounced in Silicon-On-Insulator MOSFET structures due to the low thermal conductivity of the insulating buried oxide (1.4W/mK compared to 148 W/mK for silicon). This leads to reduction in the device current and a negative output conductance.

In this paper, an analysis of the effect of the self-heating on the gate transconductance (gm) is presented. This analysis includes the reduction of the carrier mobility and threshold voltage with temperature. Analytical results show that when including self-heating effects, the transconductance gm is lower compared to the transconducance without self-heating. This reduction in gm is attributed to reduction in mobility and threshold voltage when self-heating effects are considered. Analytical results are verified by 2D numerical simulations of a fully-depleted SOI MOSFET structure with 0.8um channel length by use of the ATLAS/GIGA 2D simulator from SILVACO.

Simulations show that at VGS of 2.0V, device power is 0.4mW and channel temperature rise is 40C. The transconducatance (gm) drops by 14%, output conductance (gds) drops by 32.8% and device current (IDS) drops by 7% compared to their respective values without self-heating. The effect of self-heating on circuit performance is also investigated by analysing a CMOS inverter DC and AC characteristics using 2D simulations. Simulation results indicate that inverter gain is reduced at low frequencies due to self-heating effects and increases at high frequencies.

Moisture Effects on Strength Parameters of a Wood-Thermoplastic Composite Material.

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The present work investigates the effects of marine exposure environments on strength parameters of a wood-thermoplastic composite (W.P.C) under static and fatigue loading. This work is a part of the durability-modeling program of engineered W.P.Cs for the naval waterfronts.

A study of the moisture diffusion process is presented along with correlation between the diffusion data and a Fickian diffusion model. Effects of internal variables such as additives and processing methods (flat pressing, extrusion) as well as external variables such as the fluid environments (distilled, seawater) and fluid temperature on the diffusion process are examined.

Degradation of material performance due to fluid sorption is quantified by measuring the decrease in static strength and stiffness, which is indicative of sorption related material damage. Light microscope surface images of coupons subjected to these fluid environments for extended time periods reveal significant attack on the thermoplastic phase and present visual evidence of the above described material damage.

Fatigue data for the material is presented in the form of S-N curves. It is shown that the damage accompanying the cyclic loading manifests itself in the form of a reduction in the stiffness along the loading direction. This is monitored by a continuous measurement of the coupon stiffness during the fatigue life. The decreasing coupon stiffness during the fatigue life when plotted versus time enables the measurement of a damage rate. This damage rate is shown to depend on the maximum stress in the fatigue cycle.

Finally the effect of fluid exposure on cyclic loading is investigated. Saturated coupons were subjected to cyclic loading when immersed in seawater. It is shown that during immersed fatigue, fluid transport into the coupon occurring by both capillary action through the surface pores and microcracks as well as by the diffusion process, reduce the fatigue life of the material. This degraded fatigue performance under immersed conditions can be measured in terms of an increased damage rate.

Second-Order Estimates For The Effective Behavior Of Particle-Reinforced Rubbers

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The prediction of the effective constitutive properties of composite materials is a fundamental problem in the field of mechanics of materials. Homogenization theory constitutes a useful tool in this respect since it allows the characterization of the overall, large-scale behavior of composite materials. The theory is fairly well developed for linear composites, including different approaches to the problem with varying degrees of mathematical sophistication. By contrast, the study of composite materials with nonlinear (finite) elastic phases has not been developed to the same extent, presumably because of the intrinsic difficulties associated with the geometrical and constitutive nonlinearities involved. Examples of such material are carbon-black filled elastomers, widely used in the tire manufacturing industry. Knowledge of the overall stress and strain fields, especially at large deformation, is a key component in the understanding of critical processes such as elastomer-filler debonding, filler aggregate breakdown and matrix degradation. This work makes use of the "second-order" procedure, developed in [1] for nonlinearly viscous materials, to define the effective energy function of the nonlinear elastic composite in terms of that of a suitably chosen linear thermoelastic composite material with the same microstructure as the nonlinear elastic one. The procedure is applied to obtain estimates of Hashin-Strikman type for particle-reinforced rubbers and the results are compared with the recent numerical results of Govindjee [2].

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Fatigue and Damage Accumulation

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It is readily observable that crack growth during fatigue occurs for values of stress intensity factor well below the fracture toughness of a material. For crack growth to occur during fatigue, some form of weakening of the material must occur. Damage accumulation is a common explanation.

Despite this, damage measurement is rarely included as part of fatigue investigation. Our introduction to the connection between damage and fatigue was partly due to previous work [1-4] suggesting that crack closure is not as dominant a factor as literature suggests. It was found that high cycle fatigue crack growth is more dependent on the material condition at the crack tip. As inferred from previous studies, for a crack to grow damage must accumulate. That is to say, a fatigue damage zone (FDZ) must exist within a plastic zone before crack growth initiates. The FDZ could be considered to be subjected to conditions akin to those of low cycle fatigue (LCF). Understanding damage accumulation during LCF is thus crucial for understanding crack growth under HCF.

This was investigated experimentally via the following procedure. Typical tensile specimens were exposed to varying degrees of LCF damage and then notches were machined into the middle of the gauge length. The specimens were then exposed to HCF loading until failure. Compliance measurements were taken at regular intervals during the HCF and LCF exposure to observe damage accumulation. The number of cycles to failure was also recorded.

Before LCF, the compliance measurement was used to calculate the Youngs modulus. Following LCF, the new Youngs modulus, E*, normalised against the virgin value, E, was used to calculate a damage parameter, cf. Lemaitre [5]:

$$D = 1 - E^*/E$$

A typical result for mild steel (AS1214) is seen in the figure with a clear indication of the accumulation of damage observable.

As can be seen in the figure, the damage parameter D increases from 0 to about 0.4 with increasing LCF exposure. Fracture of this specimen occurred at 103,000 cycles and before 100,000 cycles, no crack initiation could be seen. Damage was not confined to one area since plastic deformation was spread over the entire gauge length. However, when D reached 0.4 macro-crack initiation occurred and failure ensued within 3,000 cycles. It is postulated that a critical damage density was reached where interaction of damage resulted in macro-crack initiation. It is clearly seen that the damage accumulation process in not a linear one.

Interestingly, there is an initial number of cycles where damage is either below the sensitivity of the compliance measuring equipment or damage has not yet begun to accumulate. Previous work has demonstrated that confinement of LCF cycle number to within this zone can result in a dramatic increase in HCF life [3,4]. This despite the fact that the materials tested are of the cyclically softening type. Conditions that result in this increased fatigue resistance are being investigated.

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A Numerical Study of Conjugate Gradient Directions for an Ultrasound Imaging Application

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Ultrasound imaging for medical diagnosis began in the 1940s. Since that time the standard approach has been the pulse-echo technique which uses only the reflected ultrasound signal and time-of-flight to reconstruct the image of an object. In pulse-echo imaging it is assumed that scattering of the ultrasound energy can be ignored.

However, at typical imaging frequencies, 3 to 10 MHz, scattering by the object does occur and leads to poor resolution. Much better resolution can be obtained using an inverse scattering approach which, unlike the pulse-echo approach, includes scattering. In inverse scattering an image is reconstructed using measurements of the ultrasound energy at many different angles around the object so that much more physical information is obtained. However, this approach results in a ill-posed, nonlinear integral equation. The conjugate gradient (CG) method has been used to solve this integral equation, but it has been found that the choice of the conjugate gradient direction has a significant impact on performance. In this paper, we investigate the effect of using the different conjugate gradient directions known as PPR, HS, FR, YD and the two-parameter family (TPF). Each algorithm is applied to three test cases for different contrasts and phase shifts which represent the ultrasonic properties of the tissues. The higher the contrasts and phase shifts are, the more difficult it is to reconstruct the object. Initial guesses of zero are used for all the experiments--that is, no prior knowledge of the object is used. Test Case 1 has low contrast with a phase shift of 0.2pi. Reconstruction of the object is obtained for all directions. The FR gives the largest mean-square error and requires the greatest CPU time. The performances of the PPR, HS, YD, and TPF directions are comparable in terms of accuracy and CPU time. Test Case 2 has medium contrast with a phase shift of 0.75pi. The FR direction fails to reconstruct the object. However, the PPR, HS, YD, and TPF directions successfully reconstruct the object with similar mean-square-error, while the YD direction takes the least CPU time.

Test Case 3 has very high contrast with a phase shift of 1.003pi. The FR, PPR, HS, and TPF directions do not work well for this case, but the reconstruction for the YD direction is reasonably accurate. For high contrast objects prior knowledge of the object incorporated into the initial guess should improve the accuracy of the results. The CG method is also applicable to other imaging techniques, such as microwave imaging and computed tomography.

Effects Of Particle Interaction And Size Variation On Damage Evolution In Filled Elastomers

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A micromechanical analysis of damage evolution (interfacial debonding) in particle-filled elastomers addresses the effect of the interactions between particles and of variation in filler size. The composite is treated as an assembly of two constituents in a finite element model. It is shown that the interaction between particles controls the damage evolution: (1) For high volume fraction, a relatively small change in particle size has a surprisingly large effect on the local material response; (2) for large differences in particle sizes (e.g. bimodal distribution), damage occurs at interfaces between large particles and matrix, with limited damage occurring at small particles. While these effects of particle interaction and size variation are smoothed out in a large ensemble of particles, it is foreseeable that they are an important factor in a failure process such as macroscopic crack propagation, which spans scales considerably larger than the maximum particle size.

Specifically, one expects thus that in the vicinity of a macroscopic coalesce into larger ones and join up with the macro crack, while small particles operate primarily so as to locally stiffen the matrix without incurring significant damage in their vicinity.

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