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14. ABSTRACT The ARO grant provided financial support for the organization of an IUTAM Symposium on "Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions" held June 20-22, 2016 in Baltimore MD. The symposium was a huge success with attendance by prominent, internationally regarded researchers, as well as junior researchers with promise. Distinguished speakers from academia, industry and government laboratories addressed the state of the art in the thematic areas of the symposium. Various events that took place at the symposium.							
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a. REPORT	b. ABSTRACT					c. THIS PAGE	Somnath Ghosh
UU	UU	UU	UU			19b. TELEPHONE NUMBER 410-516-7833	

Report Title

Final Report: IUTAM Symposium on Integrated Computational Structure_ Material Modeling of Deformation and Failure Under Extreme Conditions

ABSTRACT

The ARO grant provided financial support for the organization of an IUTAM Symposium on “Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions” held June 20-22, 2016 in Baltimore MD. The symposium was a huge success with attendance by prominent, internationally regarded researchers, as well as junior researchers with promise. Distinguished speakers from academia, industry and government laboratories addressed the state of the art in the thematic areas of the symposium. Various events that took place at the symposium.

I. Presentations by Distinguished Speakers: A total of 34 presentations/lectures were made by distinguished researchers in complementary areas of physics-based multi-scale model development, multi-scale data acquisition and characterization, probabilistic modeling & uncertainty quantification, and experimental methods.

II. Panel Discussions by Leading Industry and Government Visionaries: 3 panel discussion sessions took place, led by key people from various industries (multi-national) and government agencies.

III. Poster session: A total of 19 posters were presented at this session.

IV. Publications: Two international journals have allocated special issues for papers presented at the IUTAM symposium.

In summary, the IUTAM symposium provided a broad, comprehensive vision to direct future research in this general field of integrated computational structure-material modeling under extreme conditions.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
-----------------	--------------

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Abstracts of presentations are provided with the report.

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received

Book Chapter

TOTAL:

Patents Submitted

N/A

Patents Awarded

N/A

Awards

N/A

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME PERCENT SUPPORTED
FTE Equivalent:
Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attachment

Technology Transfer

Technology transfer in the symposium took place through presentation and poster sessions.

**IUTAM Symposium on Integrated Computational Structure-
Material Modeling of Deformation and Failure under Extreme
Conditions**

Sponsor: Army Research Office

Program: Solid Mechanics

Agreement No. W911NF1610360

Period of Performance: 06/03/2016 - 06/02/2017

Program Director: Dr. Asher Rubinstein

By

Somnath Ghosh

Professor, Departments of Civil, Mechanical, Materials Science & Engineering

Johns Hopkins University, Baltimore, Maryland

April 2017

1. INTRODUCTION

This constitutes the final report for the ARO conference grant, entitled “IUTAM Symposium on Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions” This grant was for the period June 3, 2016 to June 2, 2016. This grant provided financial support for the organization of an International Union of Theoretical and Applied Mechanics (IUTAM) Symposium on “Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions”. Important information on the symposium is given below.

- Title:** IUTAM Symposium on “Integrated Computational Structure-Material Modeling of Deformation and Failure under Extreme Conditions”
- Location:** Royal Sonesta Harbor Court Hotel
Inner Harbor, Baltimore, Maryland, USA
550 Light Street, Baltimore MD 21202 USA
- Dates:** June 20-22, 2016
- Host:** Whiting School of Engineering, Johns Hopkins University
3400 N. Charles Street, Baltimore MD 21218 USA
- Co-Sponsor:** US Association of Computational Mechanics
- Web-sites:** <http://iutam.org/iutam-symposium-on-integrated-computational-structure-material-modeling-of-deformation-and-failure-under-extreme-conditions/>
<http://iutam2016ics.usacm.org/>

The symposium was a huge success with attendance by prominent, internationally regarded researchers, as well as junior researchers with promise. A variety of events took place at the conference. At the end, the participants decided to continue this as a biennial event that can be internationally organized. Some of the detailed of the symposium are provided next.

2. ORGANIZING/SCIENTIFIC COMMITTEE

The international organizing committee encompasses 5 countries.

- Prof. Somnath Ghosh, *Johns Hopkins University*, (**Symposium Chair**), Baltimore, MD, USA
- Dr. Curt A. Bronkhorst, *Los Alamos National Laboratories*, Los Alamos, NM, USA
- Prof. Fionn P. Dunne, *Imperial College*, London, UK
- Prof. Kevin Hemker, *Johns Hopkins University*, Baltimore, MD, USA
- Prof. Georges Cailletaud, *MINES ParisTech*, Paris, France,
- Prof. Pierre Ladeveze, *ENS Cachan*, Cachan Cedex, France
- Prof. Pedro Camanho, *University of Porto*, Porto, Portugal
- Prof. Zhuo Zhuang, *Tsinghua University*, Beijing, China

Symposium Secretariat

- Ruth Hengst: USACM Secretariat
- Khairul Bariah Abd. Majid: Johns Hopkins University Coordinator

3. SYMPOSIUM VISION

High demands on future systems in various applications are challenging the operational limits of materials like metals, ceramics and composites. Design of enhanced systems to meet performance and reliability challenges requires advanced methods of analysis and simulation to provide a comprehensive understanding of the structure-material behavior. To address these challenges, this IUTAM symposium brought together top researchers and experts from academia, government laboratories and industry all over the world to engage in a discussion on present and future directions in the multidisciplinary approaches for integrating modeling and simulation, characterization and experiments to predict non-homogeneous deformation and failure in heterogeneous materials. It focused on different material classes including metals, ceramics and composites and covered a range of spatial and temporal scales needed for physics-based modeling of deformation and failure. The symposium addressed research needs in complementary areas of: (i) physics-based multi-scale model development, (ii) multi-scale data acquisition and characterization, (iii) probabilistic modeling & uncertainty quantification, and (iv) experimental methods.

4. MAJOR EVENTS

An interdisciplinary group, ranging from specialists in Computational Mechanics, Experimental Mechanics, Materials Characterization and Data Assimilation to Uncertainty Quantification, representing a broad range of disciplines e.g. Mechanical Engineering, Civil Engineering, Materials Science & Engineering, Aerospace Engineering, Physical Sciences, etc. participated in the conference. Distinguished speakers from academia, industry and government laboratories addressed the state of the art in the thematic areas of the symposium. Various events that took place at the symposium are summarized next. The details are presented in the Appendix.

I. Presentations by Distinguished Speakers: A total of 34 presentations/lectures were made by distinguished researchers in complementary areas of physics-based multi-scale model development, multi-scale data acquisition and characterization, probabilistic modeling & uncertainty quantification, and experimental methods. The titles of their presentations and abstracts are given in the Appendix. It provided participants with a comprehensive understanding of the state of the art in these fields.

II. Panel Discussions by Leading Industry and Government Visionaries: 3 panel discussion sessions took place, led by key people from various industries (multi-national) and government agencies. A white paper is being assembled from the outcome for dissemination to various governmental agencies. These are mentioned below.

Panel 1: Linking Microstructure to Performance across Fatigue and Failure Loading Regimes in Single and Polycrystal Metal Alloys

This session addressed key microstructural features including grains, boundaries, interfaces, twins, crystallography, micro-texture, phase, and triple junctions in polycrystal slip and twinning (all where appropriate) in metals, over regimes of fatigue including classically described low, high and very high cycle loading, with particular focus on addressing mechanistic understanding and

identification of the appropriate length scale at which to seek understanding. It addressed links between mechanistic understanding and key in-service performance measures in terms of, e.g., structural integrity strength, endurance, and fatigue life. The aim of the discussion was to attempt to construct guidelines to define the fundamental research needed to address key safety critical, high-value, industrial performance needs.

Panel 2: Response of Materials to Dynamic Mechanical Loading and Their Physical Representation

The response of materials to extreme loading conditions, especially when damage and failure events occur remains a significant challenge to capture experimentally and successfully describe computationally. Many physical processes e.g. plasticity, porosity, shear banding, cleavage and delamination, involved in extreme loading of materials entail statistical distributions of properties and rare events for which our mean-value state variable theories require further development. This necessarily entails direct linkages to microstructural details of the material in question – whether metallic, ceramic, or composite. New numerical techniques must also be envisioned to enable successful representation of these discrete events which expand in size. In addition to the uncertainty in the experiment/model coupling, many conditions for which we must develop models are not approachable experimentally and therefore quantifying uncertainty in extrapolation of model use beyond experience is critical. Within the international community, new experimental capabilities are being developed or planned which will allow for *in-situ* probing of physical response taking place at small length and time scales. Close collaboration between the experimental, modeling, and simulation communities will be critical to allow for extracting of physical insights from these new types of results. This discussion attempted to construct guidelines to define the fundamental research needed to address key defense and industrial needs.

Panel 3: Radiation and High Temperature Environment Materials – Modeling and Design of Advanced Material Systems in Nuclear Environment

Materials for use in radiation and high temperature environments, which may also involve high levels of mechanical loading, are in most cases designed specifically for these types of conditions. In these cases, the coupling of modeling, simulation, and experimental results is particularly important to facilitate greater performance advancement. For these applications, mechanisms of deformation and damage with service time exposed to these conditions are also sensitive to the structure of the material and in some cases performance enhancement relies on the control of the structure or different combinations of materials. For these extreme environment conditions, mechanisms of deformation and damage are critically important to identify in order that these particular mechanisms can be controlled to delay or avoid material failure. In addition, experiments can be very difficult and sometimes impossible, then only computations are available. The computations involve much effort and further work is necessary to define multiscale and multiphysics modeling at the very small scale as well as computational techniques. Lifetime prediction is also particularly important for these applications since the cost of failure can be very high. Discussions of the coupling of modeling and experimentation to uncertainty reduction were sought. In addition, the panel defined work needed to advance our understanding of critical behavioral mechanisms for these materials.

Based on these discussions, we plan to draft a white paper for dissemination to various governmental agencies.

III. Poster session:

A poster session was held to showcase research progress made by junior researchers and to encourage them to think of the future of the field as perceived by noted leaders from various sectors. A total of 19 posters were presented at this session and details are given in the Appendix.

IV. Publications:

Two international journals have allocated special issues for papers presented at the IUTAM symposium. They are (i) Computational Mechanics and (ii) International Journal of Fracture. S. Ghosh and C. Bronkhorst are serving as the guest editors for these special issues.

V. Networking:

The symposium provided an excellent platform for networking of researchers in academia, industry and government from multiple countries, and belonging to multiple yet complementary disciplines. It also provided opportunities for junior researchers to connect with distinguished international researchers.

In summary, the IUTAM symposium provided a broad, comprehensive vision to direct future research in this general field of integrated computational structure-material modeling under extreme conditions.

The ARO grant paid for the \$500 registration fee of approximately 8 junior faculty members and for young researchers and students from academia. In addition, the grant partially covered other organizational costs such as audio visual equipment rental, poster board stands for the poster session and flip boards rentals for the discuss panels.

REGISTRATION

Registered regular from the USA:	53
Registered student attendees from the USA:	21
Total registered US based attendees:	53
Registered regular attendees from outside the USA:	17
Total registered foreign attendees:	17
Total registered attendees:	91

Appendix I

Symposium Schedule

Monday, June 20

Whitehall Ballroom

7:00 am – 8:00 am

Continental Breakfast

7:15 am

Registration and check-in opens

8:00 am

Welcome Remarks

Session 1

Chair: Curt Bronkhorst

8:30 am – 9:00 am

D. McDowell (Georgia Institute of Technology), *Multiscale Crystal Plasticity Modeling for Metals under Extreme Conditions*

9:00 am – 9:30 am

W. Curtin (Ecole Polytechnique Federale de Lausanne), *Design of Ductility Starting from First-Principles*

9:30 am – 10:00 am

F. Dunne (Zebang Zhen Imperial College), B. Britton, D. Balint, P. Ashton, M. Cuddihy, T. Jun, Z. Zhang, Z. Zheng, *Dwell Fatigue in Titanium Alloys: An Assessment of Rate Sensitivity, Temperature, Morphology and Stress State*

10:00 am – 10:30 am

R. Lebensohn (Los Alamos National Laboratory), R. Pokharel, *Towards an Integrated Experimental/Modelling Framework to Account for Microstructural Effects on Damage under Extreme Conditions*

Session 2

Chair: Fionn Dunne

10:45 am – 11:15 am

T. Pollock (University of California, Santa Barbara), M. Echlin, W. Lenthe, *Acquisition and Analysis of 3D Mesoscale Microstructural Information for Property Modeling*

11:15 am – 11:45 am

K. Ravi-Chandar (University of Texas at Austin), A. Gross, *On the Deformation and Failure of AL 6061--T6 Evaluated through In Situ Microscopy*

11:45 am – 12:15 pm M. Uchic (AFRL), M. Groeber, J.M. Scott, *Efficient 3D Characterization of Titanium Microstructures via Serial Sectioning Combined with Correlative Microscopy Methods*

Session 3

Chair: K. Ravi-Chandar

1:30 pm – 2:00 pm K. Hemker (Johns Hopkins University), *Underpinning and Benchmarking Multi--Scale Models with Micro--Scale Experiments: An Experimentalist's Perspective*

2:00 pm – 2:30 pm C. Woodward (Air Force Research Laboratory), S.I. Rao, A. Hussein, B. Akdim, E. Antillon, D. Dimiduk, *Intrinsic Deformation Scale--Effects in Metals*

2:30 pm – 3:00 pm H. Waisman (Columbia University), *A Unified Model for Metal Failure Capturing Shear Banding and Fracture*

3:00 pm – 3:30 pm F. Pires (University of Porto), I. Lopes, *Analysis of the Deformation Behaviour of Ductile Materials with Parallel Homogenization--Based Multiscale Strategies*

3:30 pm – 4:00 pm J. El-Awady (Johns Hopkins University), *Large--Scale Dislocation Dynamics Simulations of Plasticity and Point Defect Evolution in Persistent Slip Bands*

4:00 pm – 4:15 pm Afternoon Break/Poster Viewing (Whitehall Ballroom)

Panel 1: Metals/Fatigue/Failure Discussions (Industry & Government)

4:15 pm – 5:45 pm D. Rugg, *Rolls Royce*, D. Furrer, *Pratt & Whitney*

Posters available for viewing after 5:45 pm until 6:30 pm.

Tuesday, June 21

Whitehall Ballroom

7:00 am – 8:00 am

Continental Breakfast

Session 4

Chair: Kevin Hemker

8:00 am – 8:30 am

A. Wilkinson (University of Oxford), J. Gong, T. Britton,
*Experimental Analysis of Material Deformation at the Micro- and
-Meso Scales*

8:30 am – 9:00 am

A. Rollett (Carnegie Mellon University), E. Lieberman, R.
Lebensohn, C. Bronkhorst, *Microstructural Effects on Damage
Evolution in Shocked Copper Polycrystals*

9:00 am – 9:30 am

K.T. Ramesh (Johns Hopkins University), *The Secret Lives of
Twins*

9:30 am – 10:00 am

Z. Zhuang (Tsinghua University), Z. Liu, Y. Cui,
*Discrete Dislocation--Based Crystal Plasticity at Submicron
Scale*

10:00 am – 10:15 am

Morning Break/ Poster Viewing (Whitehall Ballroom)

Session 5

Chair: Xin Sun

10:15 am – 10:45 am

J. Bassani (University of Pennsylvania),
Strain Localization in the Presence of Microstructural Evolution

10:45 am – 11:15 am

J. Clayton (U.S. Army Research Laboratory--Aberdeen),
*A Finsler Differential--Geometric Description of Deformable
Solids with Microstructure*

11:15 am – 11:45 am

P. Wriggers (Leibniz University Hannover), S. Zeller, S.
Loehnert, *A Multiscale Approach for Modeling Thermoplastic
Thermal Behaviour of Dual--Phase Steels*

11:45 am – 12:15 pm

R. Becker (U.S. Army Research Laboratory--Aberdeen),
*Determination of Spall Sensitivity to Matrix Material
Properties by Direct Numerical Simulation*

12:15 pm – 1:30 pm

Lunch – Brightons Room

Session 6

Chair: Zhuo Zhuang

- 1:30 pm – 2:00 pm C. Bronkhorst (Los Alamos National Laboratory), H.M. Mourad, V. Livescu, E.K. Cerreta, D.J. Luscher, J.R. Mayeur, G.T. Gray, III, *Prediction and Numerical Representation of Adiabatic Shear Banding in Metals*
- 2:00 pm – 2:30 pm J-S. Chen (University of California, San Diego), S. Lin, *A Stochastic Damage Analysis for Brittle Materials and its Application to Fragment--Impact Modeling of Concretes*
- 2:30 pm – 3:00 pm S. Mahadevan (Vanderbilt University), *Uncertainty Integration across Multiple Levels for Structure--Material Performance Assessment*
- 3:00 pm – 3:30 pm S. Ghosh (Johns Hopkins University), *Computational Mechanics in Advancing the Integrated Computational Materials Science & Engineering (ICMSE) Initiative for Metals and Alloys*
- 3:30 pm – 4:00 pm Afternoon Break/Poster Viewing (Whitehall Ballroom)

Panel 2: Dynamics Discussions (Industry & Government)

- 4:00 pm – 5:30 pm M. Schraad, *Los Alamos National Laboratory*, S. Schoenfeld, *Army Research Laboratory*, C. Przybyla, *Air Force Research Laboratory*

Posters available for viewing after 5:30 pm until 6:30 pm.

- 7:00 pm Banquet - Brightons Room

Wednesday, June 22

Whitehall Ballroom

7:00 am – 8:00 am

Continental Breakfast

Session 7

Chair: Suvranu De

8:00 am – 8:30 am

P. Ladeveze (LMT Cachan- ENS Cachan, CNRS, Université Paris-Saclay), D. Neron, H. Bainier, *An Integrated Computational Material--Structure Modeling for Laminated Composites*

8:30 am – 9:00 am

G. Lubineau (King Abdullah University of Science and Technology), *Challenges in Engineering Composites: Predictive Design, Joining Strategy and Structural Health Monitoring*

9:00 am – 9:30 am

S. Kruch (Onera – The French Aerospace Lab), D. Boivin, N. Horezan, P. Kanouté, Y. Renollet, *Multi--Scale Microscopy Applied for Material Characterization*

9:30 am – 10:00 am

B. Cox (Arachne Consulting), *Stochastic Aspects of High Fidelity Discrete Cracking Simulations*

10:00 am – 10:15 am

Morning Break

Session 8

Chair: Pierre Ladeveze

10:15 am – 10:45 am

P. Camanho (Universidade do Porto), R. Tavares, A. Turon, G. Catalanotti, M. Bessa, *Development of Non--Conventional Composite Materials*

10:45 am – 11:15 am

S. De (Rensselaer Polytechnic Institute), *Jacobian--Free Multiscale Methods (JFMM): Application to Radiation Damage*

11:15 am – 11:45 am

A. Cocks (University of Oxford), *Modelling Damage Development and Crack Growth in Welded Components*

11:45 am – 12:15 pm

P. Geubelle (University of Illinois), C. Zhang, J. Sung, N. Sottos, *Dynamic Spallation of Film/Substrate Interfaces Tailored with Self Assembled Monolayers: A Multiscale Model of Interface Roughness Effect*

Appendix II

Posters session (Monday, June 20 and Tuesday, June 21)

A.1. **Prof. Reza Abedi**, *University of Tennessee*

“Probabilistic Fracture Modeling of Quasi-Brittle Materials using an Interfacial Damage Model”

A.2. **Dr. Coleman Alleman**, *Sandia National Labs*

“Concurrent Multiscale Modeling of Microstructural Effects on Localization Behavior in Finite Deformation Solid Mechanics”

A.3. **Dr. T. Ben Britton**, *Imperial College London*

“The Power of Correlative Microscopy--Understanding Deformation Compatibility with HR-EBSD and HR-DIC”

A.4. **Prof. Yuli Chen**, *Beihang University*

"Stiffness Threshold of Carbon Nanotube Networks"

B.1. **Dr. Jiahao Cheng**, *Johns Hopkins University*

“A Novel CPFE Model for Explicit Twin Formation and Deformation Heterogeneity in Magnesium Polycrystalline Microstructure”

B.2. **Dr. Christoph Eberl**, *Fraunhofer Institute for Mechanics of Materials IWM*

"Experimental Investigation of Crack Initiation in FCC Materials in the High and Very Cycle Fatigue Regime"

B.3. **Dr. Jake Hochhalter**, *NASA*

"Determination of Carbide Cracking Micro-mechanisms Using HR--EBSD and CP--FEM"

B.4. **Dr. Jun Jiang**, *Imperial College London*

"Understanding of Material Mechanics at Microstructural Scale"

C.1. **Prof. Marko Knezevic**, *University of New Hampshire*

"An Accurate Description of Rate--Sensitive Flow of Polycrystals across Multiple Scales"

C.2. **Prof. Antonios Kontsos**, *Drexel University*

"Microstructure--Driven Computational Modeling of Shear Bands in Mg Alloys"

C.3. **Prof. Dharendra Kubair**, *Johns Hopkins University*

“Exterior Statistics--based Boundary Conditions for Representative Volume Elements of Elastic Composites”

C.4. **Prof. Leslie Lamberson**, *Drexel University*

"Full-Field Dynamic Fracture Analysis: A Hybrid Experimental--Computational Approach"

D.1. **Prof. Zhanli Liu**, *Tsinghua University*

"Developing Microscale Crystal Plasticity Model Based on Phase Field Theory for Modeling Dislocations in Heteroepitaxial Structures"

D.2. **Dr. Stephen R. Niezgoda**, *The Ohio State University*

"Insights on Shear Band Behavior in BMGMCS from FFT-Based Continuum Modeling"

D.3. **Dr. Arun Prakash**, *Purdue University*

"Multi-scale Computational Framework for Simulation of Cellular Solids"

D.4. **Prof. Dong Qian**, *University of Texas at Dallas*

"A Multiscale Simulation Approach to Interaction of Ultra-Short Pulse Laser with Metallic Materials"

E.1. **Prof. Thomas Siegmund**, *Purdue University*

"Length scales and the Failure Analysis of Metals at High Temperatures"

E.2. **Prof. Ashley Spear**, *University of Utah*

"Integrating Data from Experiments & Simulations to Elucidate Small-Crack Growth Mechanisms"

E.3. **Prof. Mitra Taheri**, *Drexel University*

"Coupling Quantitative Dislocation Analysis with In Situ TEM: Toward Predictive Understanding of Materials at Extremes"

APPENDIX III

Abstracts of oral presentations

MULTISCALE CRYSTAL PLASTICITY MODELING FOR METALS UNDER EXTREME CONDITIONS

David L. McDowell

Woodruff School of Mechanical Engineering School of Materials Science and Engineering
500 Tenth Street, NW, PTB Building, Room 415 Georgia Institute of Technology
Atlanta, GA 30332-0620 USA
david.mcdowell@me.gatech.edu

Focus Material: Metals

Focus of the Presentation: Physics-based multi-scale model development

Abstract

Crystal plasticity modeling is useful for considering the influence of anisotropy of elastic and plastic deformation on local and global responses in crystals and polycrystals. Modern crystal plasticity has numerous manifestations, including bottom-up models based on adaptive quasi-continuum and concurrent atomistic-continuum methods in addition to discrete dislocation dynamics and continuum crystal plasticity. Some key gaps in mesoscale crystal plasticity models will be discussed, including interface slip transfer, grain subdivision in large deformation, evolution of defects and deformation in irradiated materials, shock wave propagation in heterogeneous polycrystals, and dislocation dynamics with explicit treatment of waves. Given the mesoscopic character of these phenomena, contrasts are drawn between bottom-up (simulations and experimental observations) and top-down (experimental) information in assembling mesoscale constitutive relations and informing their parameters. Owing to the high utility of metastable structures in practice, kinetic pathways for mesoscale defect structures are considered. We consider requirements for coarse-graining of microstructure evolution across scales based on the notion of spatio-temporal activation volume averaging exploiting transition state theory.

DESIGN OF DUCTILITY STARTING FROM FIRST PRINCIPLES

W. A. Curtin

*Ecole Polytechnique Federale de Lausanne
EPFL-STI-IGM-LAMMM, Station 9, 1015 Lausanne, Switzerland*

Abstract

Low ductility in Al alloys is a major barrier to their replacement of steels in automotive and other applications where failure by localization limits component design. Low ductility in Al-Mg alloys has long been associated with Dynamic Strain Aging – the material is stronger at lower strain rates, which encourages localization and instabilities – but no quantitative or predictive models exist. Here, we present a hierarchical, mechanistic, multiscale model that quantitatively predicts the ductility and enables the design of new higher-ductility alloys. The components of the model, all new to the metallurgy field, are:

- (1) first-principles solute/dislocation interaction energies for arbitrary solutes in Al;
- (2) predictive theory for solute strengthening in the absence of aging mechanisms;
- (3) atomic-scale “cross-core diffusion” mechanism of aging;
- (4) effects of cross-core diffusion on two mechanisms of dislocation strengthening;
- (5) full thermo-kinetic constitutive model for thermally-activated plastic flow;
- (6) implementation with an FEM model to predict coupon-scale response.

The model quantitatively predicts the entire scope of steady-state flow behavior as a function of strain-rate, plastic strain, temperature, and alloy composition in Al-Mg alloys, with all key inputs coming from quantum, atomistic, or dislocation-level computations. In particular, the predicted reduction in ductility of Al-Mg 5182 alloys at room temperature and strain rate of 10^{-3} /s is predicted in good agreement with experiments, tying the ductility loss directly to atomistic-scale phenomena. The model is then used to design new Al alloy compositions that have higher ductility at room temperature while maintaining the same yield and hardening behavior of the commercial alloys.

(1) Corresponding Author : Firstname Surname e-mail: william.curtin@epfl.ch.

DWELL FATIGUE IN TITANIUM ALLOYS: AN ASSESSMENT OF RATE SENSITIVITY, TEMPERATURE, MORPHOLOGY AND STRESS STATE

Fionn Dunne, Ben Britton, Daniel Balint, Patrick Ashton, Mitch Cuddihy,
Terry Jun, Zhen Zhang

Zebang Zheng Imperial College, Exhibition Road, London SW7 2AZ

Abstract

It is well known that alloy Ti-6242 shows a significant reduction in fatigue life, termed dwell debit, if a stress dwell is included in the fatigue cycle whereas Ti-6246 does not; the mechanistic explanation for these differing dwell debits in these alloys has remained elusive. It has been argued that thermal activation for the escape of pinned dislocations [1] is the driver for the remarkable rate sensitivity displayed by Ti alloys even at low ($<20^{\circ}\text{C}$) temperature, and crucial to dwell fatigue. Other important factors remain crystallographic orientation of rogue grain pairs, alpha-beta morphology, the intrinsic rate sensitivities of the alpha and beta phases [2], temperature [3], and the stress state.

This paper presents an assessment of the key drivers for dwell fatigue crack nucleation utilizing recent crystal plasticity and new rate-sensitive discrete dislocation plasticity modelling integrated where possible with micromechanical pillar testing and characterization. It is shown that the intrinsic material rate sensitivity, and how it manifests itself over regimes of strain rate and temperature, is the key to mechanistic understanding and provides the explanation for the temperature sensitivity in dwell, its stress state dependence, and why Ti-6242 shows a strong dwell debit whereas Ti-6246 does not. Morphological alpha-beta effects are considered and shown to be second order in dwell and the primary driver to remain the crucial alpha-phase soft-hard grain orientation combination and the resulting load shedding. It is argued that the key physical phenomenon controlling all of the above behavior is the time constant associated with the thermal activation of dislocation escape with respect to that for the loading regime.

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TOWARDS AN INTEGRATED EXPERIMENTAL/MODELLING FRAMEWORK TO ACCOUNT FOR MICROSTRUCTURAL EFFECTS ON DAMAGE UNDER EXTREME CONDITIONS

Ricardo A. Lebensohn¹ and Reeju Pokharel²

1. Materials Science and Technology Division, Los Alamos National Laboratory,
lebenso@lanl.gov

1. Materials Science and Technology Division, Los Alamos National Laboratory,
reeju@lanl.gov

Focus Material: Metals

Focus of the Presentation: *(i) Physics-based multi-scale model development*

Abstract

In-situ non-destructive 3-D characterization and micromechanical formulations that can use direct input and be validated by those emerging methods are enabling the discovery and modelling of microstructural effects on mechanical behavior of polycrystalline materials.

In this talk we report the synergistic combination of Fast Fourier Transform-based methods (e.g. [1]), which can efficiently use the voxelized microstructural images of heterogeneous materials as input to predict their micromechanical response, and High Energy Diffraction Microscopy (HEDM) (e.g. [2]) and tomography obtained in metallic aggregates developing porosity during plastic deformation that allowed us to study how microstructure affects ductile damage in these materials.

While the present experimental/modelling framework is adequate to study processes occurring at relatively low strain-rates, efforts towards extending it to dynamics extremes will be described.

References

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[2] Pokharel R., Lind J., Li S.F., Kenesei P., Lebensohn R.A., Suter R.M. and A.D. Rollett, 2015, "In-situ observation of bulk 3-D microstructure evolution of polycrystalline Cu using synchrotron radiation". *Int. J. Plasticity* **67**, pp. 217-234.

ACQUISITION AND ANALYSIS OF 3D MESOSCALE MICROSTRUCTURAL INFORMATION FOR PROPERTY MODELING

McLean Echlin, Will Lenthe, and Tresa M. Pollock
Materials Department, University of California Santa Barbara

Abstract

The development of high fidelity material property and life prediction models often requires three-dimensional information on the distribution of phases, grains or extrinsic defects across a broad range of materials systems. Acquisition of this information in appropriate representative volume elements ultimately limits the use of many conventional tomography techniques. Rapid generation of 3D mesoscale datasets with multiple channels of high-resolution information using a Tri Beam tomography platform will be discussed. The high pulse frequency (1 kHz) of ultra-short (150 fs) laser pulses can induce layer-by-layer material ablation with virtually no thermal damage to the surrounding area. The TriBeam platform has been employed to gather mm³-scale datasets for metallic, polymer, ceramic and composite materials. Challenges in the acquisition, reconstruction and analysis of these 3D datasets will be addressed. The specific problem of fatigue crack initiation in a polycrystalline nickel-base alloy and the need for 3D data will be discussed. Digital image correlation combined with tomography has revealed the nature of the microstructural "neighborhoods" that result in fatigue crack initiation.

ON THE DEFORMATION AND FAILURE OF AL 6061-T6 EVALUATED THROUGH IN SITU MICROSCOPY

Andrew J Gross¹ and Krishnaswamy Ravi-Chandar²

1. Harvard University, e-mail: andrew.gross3@gmail.com

2. University of Texas at Austin, e-mail: ravi@utexas.edu

Focus Material: Metals

Focus of the Presentation: Choose one.

- (i) *Physics-based multi-scale model development;*
- (ii) *Multi-scale data acquisition, characterization and experiments at different scales;*
- (iii) *Probabilistic modeling & uncertainty quantification;*
- (iv) *structure-material integration and design.*

Abstract

Modeling of the inelastic response of metallic materials is of significant interest in applications in the aerospace, automobile, and naval industries. These models must encompass large inelastic deformations leading up to failure. While there are numerous investigations that postulate and implement micromechanical damage models such as the Gurson model to capture material degradation, there are very few investigations that provide quantitative experimental evaluation, both for calibration and for use structural applications. In this presentation, we provide a quantitative examination of the underlying deformation and failure mechanisms through a detailed, multiscale investigation of the deformation and failure processes in Al 6061-T6. Specifically, we utilize an in-situ loading stage in a scanning electron microscope and monitor both the macroscopic response and the local deformation and failure at high spatial resolution, identifying and quantifying the development of discontinuous deformation gradients both within grains and at grain boundaries [1]. The deformation and microstructural changes leading up to failure within the localized bands are identified, and the strain at the onset of final failure is determined at different (low) triaxiality levels. Issues related to homogenization of strain, representation and calibration of phenomenological plasticity, and mechanisms of failure will be discussed.

References

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EFFICIENT 3D CHARACTERIZATION OF TITANIUM MICROSTRUCTURES VIA SERIAL SECTIONING COMBINED WITH CORRELATIVE MICROSCOPY METHODS

Michael Uchic¹, Michael Groeber¹ and J. Michael Scott²
¹Air Force Research Laboratory; ²UES, Inc.

Abstract

The 3D quantification of titanium alloy microstructures-especially at scales which are relevant for engineering applications-remains a technical challenge for the materials characterization community. Over the past five years, some of the present authors have conceived and developed a multi-modal characterization system that enables automated collection of electron-optic and light microscope data from metallographically-prepared samples that are approximately 30 mm in diameter. In this presentation, we highlight emerging pathways for efficient data collection for titanium alloys via the fusing and subsequent analysis of high spatial-resolution image data with electron backscatter diffraction maps collected at lower resolution. Examples of fusing both backscattered electron and optical images will be shown, for both model single-phase and two-phase engineering alloys that have been examined by the aforementioned automated characterization system.

UNDERPINNING AND BENCHMARKING MULTI-SCALE MODELS WITH MICRO-SCALE EXPERIMENTS: AN EXPERIMENTALIST'S PERSPECTIVE

Kevin Hemker hemker@jhu.edu

Focus Material: Metals

Focus of the Presentation: Multi-scale data acquisition, characterization and experiments at different scales

Abstract

Multi-scale mechanical response models depend on detailed characterization and experimental benchmarks obtained at salient length scales. Traditional methods for model validation fail to capture the underlying microstructural dependence needed to develop physics-based models. In the current study, microtensile samples have been extracted and shaped from polycrystalline Rene 88DT and are being used to elucidate underlying microstructure-property relations. These scale-specific experiments facilitate integration of mechanical response with key microstructural features (grain size, shape, orientation, etc.) of a finite number of grains that are tractable in crystal plasticity modeling. In a parallel study, the effect of local microstructure on fatigue damage has been ascertained by resonance fatigue testing of miniaturized specimens in a novel micro-bending fatigue setup. Insights on how local microstructure (grain size, shape, orientation and neighborhood) influence local plasticity and subsequent crack formation have been collected and shown to involve: slip initiation on $\{111\}$ planes, micro-crack nucleation in large grains along, but not at, the twin boundaries experiencing high resolved shear stress and elastic incompatibility, and short crack growth along $\{111\}$ planes in neighboring grains. In both sets of experiments, quantifying the microstructural dependent mechanical response of oligocrystals opens a valuable pathway for model development and validation.

INTRINSIC DEFORMATION SCALE-EFFECTS IN METALS

C. Woodward¹, S.I. Rao², A. Hussein¹, B. Akdim¹, E. Antillon¹, D.M. Dimiduk³

1. Air Force Research Lab, Wright Patterson AFB, Ohio, USA,

christopher.woodward@us.af.mil

2. École Polytechnique Fédérale, Lausanne, Switzerland, satish.rao@epfl.ch

3. Blue Quartz Software, Springboro, Ohio, USA, dmdimiduk@gmail.com

Focus Material: Metals

Focus of the Presentation: *(i) Physics-based multi-scale model development*

Abstract

Several advances in computational mechanics methods are required to realize the goals of Integrated Computational Materials Science and Engineering. These include proper multi-scale representation of material heterogeneities as well as corresponding, characteristic length-scales. Scale effects can be quantified and validated using lower scale, physics-based models. These can be systematically verified experimentally to develop scale dependent analysis methods to inform modeling of microstructure heterogeneities. Recent experiments have shown strong size effects in metal micro-pillars with dimensions below ~100 micro-meters. This size dependent behavior is consistent with deformation occurring below a characteristic dislocation correlation length. Micro-scale dislocation evolution simulations exhibit the same behavior and reveal the mechanistic source of strengthening (and stochastic flow) at these scales. In this work, large scale atomistic and dislocation dynamics simulations are used to assess the aspects of ensemble hardening in simple metals. Atomistic simulations illustrate the effects of cross slip on full 3-d simulations of forest hardening. The work hardening rates of micro pillars, uniaxial loaded along $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$, are calculated using dislocation dynamics simulations. Simulations include dislocation intersection cross slip which enhances the rapid increase in dislocation density. Analyses of the evolving dislocation ensembles, including the formation of strong dislocation heterogeneities are reviewed.

A UNIFIED MODEL FOR METAL FAILURE CAPTURING SHEAR BANDING AND FRACTURE

Haim Waisman

Department of Civil Engineering and Engineering Mechanics, Columbia University, New York, NY 10027,
waisman@civil.columbia.edu

Focus Material: Metals

Focus of the Presentation: *(i) Physics-based multi-scale model development;*

Abstract

Dynamic fracture of metals may be brittle or ductile depending on factors such as material properties, loading rate and specimen geometry. At high strain rates, a thermo plastic instability known as shear banding may occur, which typically precedes fracture. A thermodynamically consistent model which accounts for both shear banding and dynamic fracture and can thus capture both failure modes at intermediate strain rates, is proposed. The model consists of an elastic-viscoplastic material with strain hardening, strain rate hardening, and thermal softening. Fracture is modeled with the phase field method, for which a novel modification is presented here to account for the creation of fracture surfaces by inelastic work.

In this presentation I will focus on model derivation, implementation and stability analysis to determine the onset of shear or fracture localization, based on a linear perturbation analysis. Numerical results will be presented to illustrate the predictive capabilities of the unified model and the stability criterion obtained.

References

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- [2] McAuliffe C. and Waisman H., 2016, "A coupled phase field shear band model for Ductile-Brittle transition in notched plate impacts," *Computer Methods in Applied Mechanics and Engineering*, 305:173–195.
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ANALYSIS OF THE DEFORMATION BEHAVIOUR OF DUCTILE MATERIALS WITH PARALLEL HOMOGENIZATION-BASED MULTISCALE STRATEGIES

F.M. Andrade Pires¹ and I.A.R. Lopes²

1. Department of Mechanical Engineering, Faculty of Engineering, University of Porto, Portugal, fpires@fe.up.pt
2. Department of Mechanical Engineering, Faculty of Engineering, University of Porto, Portugal, ilopes@fe.up.pt

Focus Material: Metals

Focus of the Presentation: *Multi-scale data acquisition, characterization and experiments at different scales*

Abstract

The modelling of ductile heterogeneous multi-phase materials has been a topic of extensive research over recent years. An important class of computational homogenization techniques, where the influence of the underlying microstructure is explicitly accounted for in the resulting macroscopic response, is known as coupled multi-scale finite element modelling or FE². This approach is based on the nested solution of boundary value problems of two coupled scales.

Although this modelling framework enables a more accurate description of material and structural behaviour, the significant computational requirements limit its applicability. Several strategies have been proposed to overcome this shortcoming and allow to perform realistic analyses, such as parallel computing, which exploits modern computer architectures. Multi-scale models are indeed well suited for the introduction of computational parallelism. Macroscopic domain decomposition [1] and master-slave schemes [2] have been used in this context.

In the present contribution, the deformation behaviour of ductile materials is analysed with a coupled multi-scale framework where two distinct parallelization strategies are critically assessed. The first is based on a master-slave scheme, which includes load balancing, and the second employs a non-conforming domain decomposition method at the macro-scale. The relative merits of each strategy will be highlighted.

References

- [1] Feyel, F., & Chaboche, J. (2000). FE² multiscale approach for modelling the elastoviscoplastic behaviour of long fibre SiC/Ti composite materials. *Computer Methods in Applied Mechanics and Engineering*, 183, 309–330.
- [2] Matsui, K., Terada, K. & Yuge, K. (2004). Two-scale finite element analysis of heterogeneous solids with periodic microstructures. *Computers & Structures*, 82, 593–606.

LARGE SCALE DISLOCATION DYNAMICS SIMULATIONS OF PLASTICITY AND POINT DEFECT EVOLUTION IN PERSISTENT SLIP BANDS

Jafaar El-Awady

Johns Hopkins University, jelawady@jhu.edu

Abstract

One of the common dislocation microstructures forming during cyclic loading of face centered cubic metals are persistent slip bands (PSBs). Over the years, many experimental, theoretical, and computational studies have led to significant understanding of plasticity in PSBs, however, many open questions still remain in the prediction of the formation and evolution of these complex dislocation structure. In this work, large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations are performed to study dislocation plasticity and point defect evolution in PSBs in single-slip oriented nickel single crystals. In these simulations partially developed PSB structures are introduced into the simulation cell and fully reversible loading is imposed. The maximum stress of the hysteresis loops and the local dislocation density in the channels/walls are shown to increase with increasing loading cycle. The dislocation interactions in the channels and the 3D contours of the local shear stress within the channels as a function of distance from the PSB walls are characterized to reevaluate the composite model proposed by H. Mughrabi and the bowing and passing model by L.M. Brown. In addition, the spatio-temporal point defect (vacancies and interstitials) generation and evolution is quantified as a function of the dislocation density in the PSB channels and walls. The results are discussed in view of a point defect diffusion model to study their migration rates to the surface. Finally, the PSB interaction with the free surface and the surface roughness evolution are also quantified.

EXPERIMENTAL ANALYSIS OF MATERIAL DEFORMATION AT THE MICRO- AND MESO- SCALES

Angus J Wilkinson¹, Jicheng Gong², T Ben Britton³

1. Department of Materials, University of Oxford, angus.wilkinson@materials.ox.ac.uk
2. Department of Materials, University of Oxford, Jicheng.gong@materials.ox.ac.uk
3. Department of Materials, Imperial College London, b.britton@imperial.ac.uk

Focus Material: Metals

Focus of the Presentation:

(ii) Multi-scale data acquisition, characterization and experiments at different scales;

Abstract

The last decade has seen considerable advances in methods at the micro- and meso-scale for characterizing the response of metallic alloys to mechanical stimuli. A wealth of small-scale mechanical testing methods have emerged; often facilitated by focused ion beam instruments to machine small test-pieces at selected microstructural features and nano-indenters with the sensitivity to test them. At the same time spatially resolved electron and X-ray methods for characterizing stress, strain and dislocation density variations at the meso-scale have been developed. There is great synergy between these experimental advances and those being made in physically-based micro-mechanical modelling.

Examples will be given from our work on micro-cantilever testing which we have used to isolate different slip systems in hcp metals and extract critical resolved shear stress values which can then be used with crystal plasticity finite element simulations of polycrystal behaviour [1]. A recent extension of quasi-static cantilever testing to dynamical excitation for probing (very) high cycle fatigue properties will be described.

The high angular resolution electron backscatter diffraction (HR-EBSD) method for mapping lattice strain and rotation variations will also be described. Its utility will be illustrated by examining statistical variations in stress and dislocation density in relation to position in the microstructure [2].

References

- [1] Gong J, Britton TB, Cuddihy MA, Dunne FPE, Wilkinson AJ, 2015, “ $\langle a \rangle$ Prismatic, $\langle a \rangle$ basal, and $\langle c+a \rangle$ slip strengths of commercially pure Zr by micro-cantilever tests”, *Acta Materialia* **96**, pp. 249-257.
- [2] Jiang J, Britton TB, Wilkinson AJ, 2015, “Evolution of intragranular stresses and dislocation densities during cyclic deformation of polycrystalline copper”, *Acta Materialia* **94**, pp. 193-20.

MICROSTRUCTURAL EFFECTS ON DAMAGE EVOLUTION IN SHOCKED COPPER POLYCRYSTALS

E.J. Lieberman^{1,2}, R.A. Lebensohn², C.A. Bronkhorst³, A.D. Rollett¹

1. Department of Materials Science and Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, PA 15213, USA
2. Materials Science and Technology Division, Los Alamos National Laboratory, MS G755, Los Alamos, NM 87455, USA
3. Theoretical Division, Los Alamos National Laboratory, MS B216, Los Alamos, NM 87455, USA

Focus Material: Metals

Focus of the Presentation: *Physics-based multi-scale model development*

Abstract

Three-dimensional crystal orientation fields of a copper sample, characterized before and after shock loading using High Energy Diffraction Microscopy (HEDM), are used for input and validation of direct numerical simulations using a Fast Fourier Transform (FFT)-based micromechanical model. The locations of the voids determined by X-ray tomography in the incipiently-spalled sample, predominantly found near grain boundaries, were traced back and registered to the pre-shocked microstructural image. Using FFT-based simulations with direct input from the initial microstructure, micromechanical fields at the shock peak stress were obtained. Statistical distributions of micromechanical fields restricted to grain boundaries that developed voids after the shock are compared with corresponding distributions for all grain boundaries. Distributions of conventional measures of stress and strain (deviatoric and mean components) do not show correlation with the locations of voids in the post-shocked image. Neither does stress triaxiality, surface traction or grain boundary inclination angle, in a significant way. On the other hand, differences in Taylor factor and accumulated plastic work across grain boundaries do correlate with the occurrence of damage. Damage was observed to take place preferentially at grain boundaries adjacent to grains having very different plastic response.

THE SECRET LIVES OF TWINS

K.T. Ramesh¹

1. Johns Hopkins University, Baltimore, MD 21218; Ramesh@jhu.edu

Focus Material: Metals

Focus of the Presentation:

(i) Multi-scale data acquisition, characterization and experiments at different scales

Abstract

Deformation twinning is an important deformation mechanism in a variety of materials, including metals and ceramics. This mechanism is particularly important in HCP metals and in BCC metals at high rates of deformation. We focus here on the dynamics of twinning through fundamental experiments and simple modeling, examining twinning in magnesium (Mg). Extension twins in Mg can accommodate significant plastic deformation as they grow, and thus twinning affects the overall rate of plastic deformation. We perform impact and high-strain-rate experiments on single crystals of Mg, and use high-speed imaging at 5 million frames per second to capture in situ the development of twinning modes. The velocities of the twins are thus obtained through direct real-time observations. Electron back-scattered diffraction is then used to characterize the nature of the twins and the microstructural evolution. Through these approaches we describe the dynamics of twinning and then seek to clarify the associated kinetics.

DISCRETE DISLOCATION-BASED CRYSTAL PLASTICITY AT SUBMICRON SCALE

Zhuo Zhuang, Zhanli Liu and Yinan Cui

AML, School of Aerospace Engineering, Tsinghua University, Beijing 100084, China,
zhuangz@tsinghua.edu.cn

Focus Material: Metals

Focus of the Presentation: (i) *Physics-based multi-scale model development;*

Abstract

Crystal plasticity at micron-nano scales involves many interesting issues. Some results are obtained for uniaxial compression experiments conducted on FCC single crystal micro-pillars, e.g. size effect and strain burst, etc. In the experiments, the mobile dislocations may escape from the free surface leading to the state of dislocation starved whereby an increase applied stress is necessary to nucleate or activate new dislocation sources. By performing in-situ TEM, the dislocation motion affected the material properties is observed. However, the atypical plastic behavior at submicron scales cannot be effectively investigated by either traditional crystal plastic theory or molecule dynamics simulation. The surfaces are transmissible and loading gradients are absent. Therefore, the strain gradient theory could not well explain these new mechanical behaviors. This in turn has led to develop new analytic and numerical models. Accordingly, a three dimensional discrete-continuous crystal plastic model is developed, which is coupling the discrete dislocation dynamics with finite element method [1]. Three kinds of plastic deformation mechanisms for the single crystal pillar are investigated: (1) Single arm dislocation source controlled plastic flow; (2) Confined plasticity in coated pillars [2]; (3) Dislocation starvation under low amplitude cyclic loadings. The predicted results agree well with the experimental data.

References

- [1] Cui Y.N., Liu Z.L. and Zhuang Z., 2015, "Theoretical and numerical investigation on confined plasticity in coated pillars at microscale. *J. Mech. Phys. Solids*, 76, 127-143
- [2] Wang Z.J., Li Q.J., Cui Y.N., Liu Z.L., Ma E., Li J., Sun J., Zhuang Z., Dao M., Shan Z.W., Suresh S., 2015, "Cyclic deformation leads to defect healing and strengthening of small-volume metal single crystals". *PNAS*, 10/14/1518200112

STRAIN LOCALIZATION IN THE PRESENCE OF MICROSTRUCTURAL EVOLUTION

John L. Bassani

Department of Mechanical Engineering and Applied Mechanics University of
Pennsylvania, Philadelphia, PA

A model is developed for a class of anisotropic elastic-plastic solids in which the orthotropic triad that characterizes the symmetry of the microstructure evolves with deformation. Microstructural spin is defined to be the difference between the material spin and plastic spin, which leads to a key relationship between plastic rate of stretching and plastic spin (derived rigorously from representation theory for tensor-valued functions). As a consequence, microstructural evolution arises from non-coaxiality between the plastic rate of stretching and the orthotropic axes, which intuitively makes sense. The resulting phenomenological theory extends classical theories of plasticity to include the evolution of the axes of material symmetry that evolve with large strain deformation. Comparisons with experimental data for polycrystals undergoing non-coaxial deformations are excellent. For loading in the plane of a textured sheet or for axial loading of a thin tube, only 2 additional material parameters are required for stressing in one of orthotropic symmetry planes. Predictions for necking, shear banding, and buckling display significant effects of microstructural evolution on strain localization. One important application of current interest arises in automotive “light-weighting” in predicting limits to sheet metal forming in Al- and Mg-alloys. Detailed simulations that include microstructural evolution in tube crushing, which show promise in developing new design concepts.

A FINSLER DIFFERENTIAL-GEOMETRIC DESCRIPTION OF DEFORMABLE SOLIDS WITH MICROSTRUCTURE

John D. Clayton ^{1,2,3}

¹Impact Physics, US ARL, Aberdeen, MD; john.d.clayton1.civ@mail.mil

²University of Maryland, College Park, MD; jdclayt1@umd.edu

³Courant Institute of Mathematical Sciences, New York, New York

Focus Material: Other

Focus of the Presentation: *Physics-based multi-scale model development*

Abstract

Finsler differential geometry is used to construct a new theory of mechanics of solid materials broad enough to encompass various metals and ceramics, both crystalline and amorphous. The general model accounts for finite deformation [1,2], nonlinear elasticity [1], and microstructural heterogeneities such as structural defects, including cracks, shear bands, twins, and/or dislocations [1]. The general kinematic structure of the theory includes macroscopic and microscopic displacement fields; the latter are represented by a state vector of (pseudo-)Finsler space. A fundamental tensor is introduced, leading to linear and nonlinear connections. An appropriate deformation gradient is newly derived via delta-differentiation of motion. Euler-Lagrange equations are derived for quasi-static equilibrium, demonstrating importance of the trace of Cartan's tensor. The new theory is invoked to describe physical problems of tensile fracture, shear localization, and cavitation. Finsler character of the metric is achieved via Weyl-type rescaling, i.e., a conformal transformation. Analytical solutions are compared to predictions of Griffith's fracture mechanics and phase field models. The new pseudo-Finsler theory is shown to encompass classical approaches: phase field solutions can be recovered when simplifying assumptions are imposed, as can other descriptions framed in Riemannian [1,2] as opposed to either Finslerian or locally Minkowskian spaces. The present solutions offer new physical insight into coupling of microscopic dilatation with fracture or slip. An increase in the Weyl parameter correlates with an increase in peak strength and energy, physically indicative of increasing slip resistance or crack surface friction coupled to microscopic dilatation. Such effects arise naturally from solution of governing equations derived via fundamental mathematical physics, without resort to ad-hoc extensions of prior theories or exercises in parameter fitting.

References

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A MULTISCALE APPROACH FOR MODELING THERMOPLASTIC MATERIAL BEHAVIOUR OF DUAL- PHASE STEELS

P. Wriggers¹ and S. Zeller¹ & S. Loehnert¹

1. Leibniz University Hannover, wriggers@ikm.uni-hannover.de

Focus Material: Metals

Focus of the Presentation: *Physics-based multi-scale model development;*

Abstract

In this work focus is placed on the development of material models for dual phase steels subjected to thermomechanical loading at finite strains. Especially the behaviour of the ferritic matrix of dual-phase steels will be investigated. Since the driving mechanisms for the plastic deformation in the ferritic phase are the formation, movement and pile-up of dislocations on preferred planes in preferred directions, many crystal plasticity models for the purely mechanical single crystal behaviour motivated by these mechanisms were proposed in the past. In this work these ideas are extended to thermomechanical material behaviour and a thermomechanical crystal plasticity model is developed for the single crystal behaviour. Attention is paid to the description of the evolution of the microstructure and its dependence on the history of deformation and on the history of temperature of the processes under consideration. Elementary processes of multiplication and annihilation of dislocations are analysed in terms of temperature and deformation rate dependence. Thermal activation is used to describe these dependences and evolution equations are postulated for the state variables describing the current dislocation structure and by this the influence of the deformation and temperature history on current material behaviour. These evolution equations and their temperature and rate dependence are crucial for the formulation of the model. Estimations of the critical resolved shear stress necessary to move dislocations through the crystal resulting from the interaction of dislocations on different slip systems and the resistance of the atomic lattice and the energy associated with a line element of a dislocation allow to formulate a thermoplastic constitutive material model for the single crystal behaviour of the ferritic phase. The developed material model will be used to simulate the material behaviour of the polycrystalline microstructure under different loading conditions.

The developed ideas and the resulting model are transferred to the macroscopic behaviour of sheet metal wrought material consisting of dual-phase steels. Within this homogenization process focus is placed on the consistency between experimental observations on a macroscopic length scale, the belonging constitutive thermoplastic material model on a macroscopic length scale and the developed material model for the single crystal behaviour. Possible forms and dependences on temperature and state variables for the macroscopic thermomechanical material model are deduced. Especially a thermodynamically consistent form for the energy stored in the material is presented

DETERMINATION OF SPALL SENSITIVITY TO MATRIX MATERIAL PROPERTIES BY DIRECT NUMERICAL SIMULATION

Richard Becker
US Army Research Laboratory, Aberdeen Proving Ground, MD 21005

Abstract

The effect of material strain hardening and strain rate sensitivity on spall response is investigated through large-scale direct numerical simulations of void growth and coalescence from 3-dimensional distributions of void nucleating particles. The computational model spans multiple particle spacings in the in-plane directions, and the finite element mesh is fine enough that several elements span the initial particle diameters in the mixed-zone Arbitrary Lagrange- Eulerian (ALE) simulations. The matrix material is represented by traditional plasticity models in which material failure is not permitted. The 1000+ particles are represented by the same material model as the surrounding matrix except the particles have low tensile strength to permit fracture, which is used to simulate particle cracking or decohesion. Voids grow and coalesce naturally in the ALE framework and the simulations produce dimpled failure surfaces similar to those observed experimentally in spalled samples. The strain hardening and strain rate sensitivity of the matrix material are altered to determine their influence on the void growth and coalescence processes and the simulated free surface velocity pull-back signal. The details available from computational model permit association of spall surface evolution with features on the free surface velocity profile.

Approved for public release; distribution is unlimited

PREDICTION AND NUMERICAL REPRESENTATION OF ADIABATIC SHEAR BANDING IN METALS

C. A. Bronkhorst¹, H. M. Mourad¹, V. Livescu², E. K. Cerreta²,
D. J. Luscher¹, J. R. Mayeur¹, G. T. Gray III²

¹Theoretical Division

²Material Science and Technology Division
Los Alamos National Laboratory
Los Alamos, NM 87545

Abstract

The high deformation rate mechanical loading of polycrystalline metallic materials, which have ready access to plastic deformation mechanisms, generally involve an intense process of several deformation mechanisms within the material: dislocation slip (thermally activated and phonon drag dominated), recovery (annihilation and recrystallization), mechanical twinning, porosity, and shear banding depending upon the material. For this class of ductile materials, depending upon the boundary conditions imposed, there are varying degrees of porosity or adiabatic shear banding taking place at the later stages of the deformation history. Each of these two processes are as yet a significant challenge to predict accurately. This is true for both material models to represent the physical response of the material or the computational framework to represent accurately the creation of new surfaces or interfaces in a mesh independent way. Within this talk, we will present an enriched element technique to represent the adiabatic shear banding process within a traditional Lagrangian finite element framework. A rate-dependent onset criterion for the initiation of a band is defined based upon a rate and temperature dependent material model. Once the bifurcation condition is met, the location and orientation of the embedded zone is computed and inserted at that Gauss point. Once embedded the boundary conditions between the localized and unlocalized regions of the element are enforced and the composite sub-grid element follows a weighted average representation of both regions. The material inside the band is able to be represented with a constitutive model independent from the outside material and the thickness of the band can be assigned by any appropriate method. In the finite strain formulation, rotation of the formed band is tracked with deformation. The process of dynamic recrystallization as an additional softening mechanism during the dynamic loading process is critical for some materials and a simple physically based representation of the structural recovery process is discussed. Both the initiation and growth of adiabatic shear banding is believed to be influenced by local structural features of a material and this talk will discuss the influence of the microstructure on this process. Experiments have been performed on 304L and 316L stainless steels and will be compared against numerical simulations to validate the performance of both the material model and computational approach. Remaining challenges will also be discussed.

A STOCHASTIC DAMAGE ANALYSIS FOR BRITTLE MATERIALS AND ITS APPLICATION TO FRAGMENT-IMPACT MODELING OF CONCRETES

Jiun-Shyan Chen¹ and Shih-Po Lin²

¹*Department of Structural Engineering, University of California, San Diego, CA*

²*Ford Motor Company, Ford Research & Advanced Engineering, Dearborn, MI*

Abstract

In this work, a micro-crack informed stochastic damage analysis is performed to consider the failures of material with stochastic microstructures. The derivation of the damage evolution law is based on the Helmholtz free energy equivalence between cracked microstructure and homogenized continuum. The damage model is constructed under the framework of stochastic representative volume element (SRVE). The characteristics of SRVE used in the construction of the stochastic damage model have been investigated based on the principle of the minimum potential energy. The mesh dependency issue has been addressed by introducing a scaling law into the derivation of damage evolution equation. The proposed methods are then applied to fragment-impact modeling of ultra-high strength concrete.

UNCERTAINTY INTEGRATION ACROSS MULTIPLE LEVELS FOR STRUCTURE-MATERIAL PERFORMANCE ASSESSMENT

Sankaran Mahadevan

Vanderbilt University, Nashville, TN, USA

sankaran.mahadevan@vanderbilt.edu

Abstract

Model-based simulation is attractive for the performance and reliability analysis of structural and material systems under extreme conditions, since full-scale testing is often unaffordable. However, model-based simulation involves many approximations and assumptions, and thus confidence in the simulation result is an important consideration in risk-informed decision-making. Sources of uncertainty are both aleatory and epistemic, stemming from natural variability, information uncertainty, and modeling approximations at multiple levels. Information uncertainty arises from sparse and imprecise data, measurement and data processing errors, and qualitative information. Model uncertainty arises due to unknown model parameters, model form assumptions, and solution approximation errors. The presentation will discuss a Bayesian framework for the aggregation of uncertainty from multiple sources towards the reliability assessment of multi-physics, multi-scale systems, linking manufacturing process to material microstructure and properties to structural performance. Multiple activities such as calibration, verification and validation are conducted as part of the model development at multiple levels, and the results of these activities need to be systematically integrated within the overall uncertainty quantification and performance prediction. In a multi-scale modeling environment, the information available is heterogeneous, from multiple sources (models, tests, experts) and in multiple formats. A systematic integration methodology of heterogeneous information using Bayesian networks will be presented. The integration of structural health monitoring information within this uncertainty quantification framework for diagnosis and prognosis of the structure and material state will be addressed. For systems with a large number of variables, scalability of the above computational methodologies is an important concern, and new strategies for computational efficiency within uncertainty aggregation will be outlined. Different analyses and tests could be performed at different levels of fidelity, offering trade-offs between accuracy and cost; thus resource allocation strategies for different uncertainty quantification activities will be outlined, and their effect on prediction confidence under extreme conditions will be studied.

COMPUTATIONAL MECHANICS IN ADVANCING THE INTEGRATED COMPUTATIONAL MATERIALS SCIENCE & ENGINEERING (ICMSE) INITIATIVE FOR METALS AND ALLOYS

SOMNATH GHOSH

Departments of Civil Engineering, Mechanical Engineering,
Materials Science & Engineering
Johns Hopkins University, Baltimore, MD 21218, USA
sghosh20@jhu.edu

Focus Material: Metals, Composites,

Focus of the Presentation: Choose one.

(i) *Physics-based multi-scale model development;*

Abstract

The Integrated Computational Materials Science & Engineering or ICMSE initiative entails integration of information across length and time scales for materials phenomena. This talk will present an integration of methods in Computational Mechanics and Computational Materials Science to address the deformation and failure characteristics of polycrystalline metals in various applications. Specifically it will address physics based modeling at different scales and multi-scale spatial (scale-bridging) and temporal modeling methods for Titanium, Magnesium and Aluminum alloys and Nickel based-superalloys. Spatial scales will range from atomistic to component levels. Application domains will include both monotonic and cyclic loading and address properties such as time and location-dependent strength, ductility and fatigue life. The talk will begin with methods of 3D virtual image construction and development of statistically equivalent representative volume element at multiple scales. Subsequently it will discuss the development of novel system of experimentally validated physics-based crystal plasticity finite element or CPFEM models to predict deformation and micro-twinning leading to crack nucleation. These CPFEM simulations will provide a platform for the implementation of physics-based crack evolution criterion that accounts for microstructural inhomogeneity. For crack evolution, a coupled molecular dynamics-continuum model for a crystalline material with an embedded crack will be discussed. A wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations will be discussed as well [1]. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods. Finally, stabilized element technology for analyzing this class of complex deformation problems will be discussed.

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AN INTEGRATED COMPUTATIONAL MATERIAL-STRUCTURE MODELING FOR LAMINATED COMPOSITES

Ladeveze Pierre , Neron David and Bainier Hadrien
LMT Cachan (ENS Cachan, CNRS, Université Paris-Saclay)
{Ladeveze, Neron, Bainier} @lmt.ens-cachan.fr

Focus Material: Composites

Focus of the Presentation: *(iv) Structure-material integration and design.*

Abstract

The last quarter-century has witnessed considerable research efforts in the mechanics of composites in order to understand and predict the behavior of these materials, the ultimate goal being the design of the materials/structures/manufacturing processes. Even in the case of laminated composites, the prediction of the evolution of damage up to and including final fracture remains a major challenge which is at the heart of today's virtual structural testing revolution engaged in by the aeronautical industry. Virtual structural testing consists, whenever possible, in replacing the numerous experimental tests used today by virtual tests.

First, the talk will emphasize our own modeling answer, and its derivation from today's understanding of the mechanisms of damage and their evolution on the micro and meso scales. The proposed multiscale damage approach is based on a Virtual Reference Material written at the microscale, with two constituents, the ply and the interface *i.e.* a material database which is also a tool for material design. Today, one tends to get a unified micromodel also involving fatigue, high-velocity, oxidation... The corner stone is a general bridge between micro- and meso-mechanics that we have built to derive the damage mesomodel used for structure computations as a homogenized model.

Finally, the current capabilities and limits of this multiscale approach are pointed out as well as computational challenges that accompany Virtual Structural Testing.

CHALLENGES IN ENGINEERING COMPOSITES: PREDICTIVE DESIGN, JOINING STRATEGY AND STRUCTURAL HEALTH MONITORING

Gilles Lubineau

King Abdullah University of Science and Technology (KAUST), Physical Science and
Engineering Division, COHMAS Laboratory, Thuwal 23955-6900, Saudi Arabia.
gilles.lubineau@kaust.edu.sa

Focus Material: Composites

Focus of the Presentation: *(i) Physics-based multi-scale model development*

Abstract

The success of continuous-fiber composites in aeronautics has inspired their use in other applications, including automotive, civil and structural engineering, and piping systems. Even so, continuous-fiber composites are not used to their full potential because (1) the relations between the microstructure and the macroscopic properties are only partially understood, (2) assembly techniques that allow better composite integration need improvement, and (3) development of methods to monitor structures made from such composites remains a challenge. Here, we review these barriers to the full use of continuous-fiber composites in materials engineering and applications and offer illustrative examples of new directions in engineering composites taken by the COHMAS Laboratory. The first example focuses on our work on predictive design of thermoplastic-laminated composites with particular application to the automotive industry. Automotive production techniques and defects differ from those in the aeronautics industry. The short design cycle in the automotive industry requires that new tools be developed that can optimize development of automotive-grade continuous-fiber tapes. The second example looks at new processing techniques that aim to improve the reliability of bonded interfaces, which are critical to achieving bolt-free solutions in civil and structural engineering applications. Our bolt-free or joining strategy relies on patterned interfaces, which can be used on previously cured laminates. Our last example considers structural monitoring. After a brief review of classical monitoring techniques, we present our monitoring strategies that are based on electrical monitoring and on clear understanding of the relations between mechanical damage and electrical properties.

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MULTI-SCALE MICROSCOPY APPLIED FOR MATERIAL CHARACTERIZATION

S. Kruch, D. Boivin, N. Horezan, P. Kanouté, Y. Renollet

Onera – The French Aerospace Lab, F-92322 Châtillon, France, serge.kruch@onera.fr,
denis.boivin@onera.fr, nicolas.horezan@onera.fr, pascale.kanoute@onera.fr,
yves.renollet@onera.fr

Focus Material: Metals

Focus of the Presentation: *Multi-scale data acquisition, characterization and experiments at different scales;*

Abstract

A new device has been developed at Onera in order to improve *in situ* mechanical tests (tension, compression, bending) and by observing at the same time local and global displacement fields. This is possible combining both observations from optical and beam electron microscopes. The optical microscope is used to observe and measure the far displacement field while the SEM focuses on specific areas allowing a higher resolution. The local and global displacement and deformation fields are measured and computed through a real-time Digital Image Correlation (DIC) acquisition system. The information acquired with this experimental device combined with non-linear finite element analyses is a new approach to propose and to identify constitutive equations for *in situ* materials which cannot be handling at the macroscopic scale. It is then possible to observe the influence and the evolution of dissipative phenomena like plasticity or damage at the microscopic scale (e.g. grains for metallic materials, fibers for composite materials). This approach has been successfully achieved for several applications like the mechanical characterization of architected microstructures or the modeling of shot peened structures.

STOCHASTIC ASPECTS OF HIGH FIDELITY DISCRETE CRACKING SIMULATIONS

Brian Cox

Arachne Consulting, Sherman Oaks, California, brian1cox@outlook.com

Focus Material: Composites

Focus of the Presentation:

(i) Physics-based multi-scale model development

Abstract

To be regarded as being faithful to reality, simulations of discrete cracking events in composites must be able to relate the stochastic variability of the material to scatter in its engineering properties, e.g., strength and fatigue life. Material variability arises in the positioning of fibers within tows or plies, as well as in the positions and shapes of tows or plies considered as homogenized entities. In recent years, new, rich sources of 3D data on material variability have inspired the generation of stochastic virtual specimens, which are calibrated by measured statistics. Calibrated virtual specimens are being generated at the fiber scale, e.g., bundles of 10^3 fibers; the tow scale, e.g., $10 - 10^2$ tows in a textile unit cell; and the sub-component scale, e.g., $10^4 - 10^6$ tow segments in an integrally woven structure [1]. Simultaneously, new formulations of fracture simulations are being sought that can deal with stochastic, multiple interacting crack systems within stochastic virtual specimens. Challenges include assuring that the physics of crack initiation, bifurcation, and coalescence is correctly represented [2] while dealing with large ensembles of virtual specimens, e.g., $10^3 - 10^4$ instantiations, that are each very large, e.g., containing by $10^8 - 10^9$ degrees of freedom.

References

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Development of Non-Conventional Composite Materials

Rodrigo P. Tavares^{1,2}, Albert Turon³, Giuseppe Catalanotti², Miguel A. Bessa⁴, and Pedro P. Camanho^{1,2}

- . 1. DEMec, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
- . 2. INEGI, Rua Dr. Roberto Frias, 400, 4200-465 Porto, Portugal
- . 3. AMADE, Polytechnic School, University of Girona, Campus Montilivi s/n, 17071 Girona, Spain
- . 4. Northwestern University, Department of Mechanical Engineering, 2145 Sheridan Rd. Evanston, IL 60208-3111

Focus Material: Composites

Focus of the Presentation: *(iv) Structure-material integration and design.*

Abstract

The need to understand the failure mechanisms in composite materials at the micro level has gained additional importance due to the increasing need to develop high performance materials for more demanding applications. This understanding makes it possible to develop new materials by recurring to hybridization, either fibre hybridization [1] or ply hybridization [2].

In this work a micromechanical model that takes into account the statistical nature of fibre strength and the fibre waviness present in composite materials is developed and used to determine the failure behaviour of hybrid and non-hybrid composite materials. The model is able to capture failure mechanisms in the three main components of a composite material: fibres, matrix and fibre-matrix interface. This study is performed for multiple load scenarios, with focus on the longitudinal tensile and compressive failure of these materials. The effect of transverse stresses in these types of failure is also assessed to better understand its effects on the failure mechanisms.

References

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JACOBIAN-FREE MULTISCALE METHODS (JFMM): APPLICATION TO RADIATION DAMAGE

Suvranu De

Rensselaer Polytechnic Institute, Troy NY; des@rpi.edu

Focus Material: Metals

Focus of the Presentation: *Physics-based multi-scale model development*

Abstract

The advantage of hierarchical multiscale methods is the ability to model arbitrary nonlinearities at the micro-scale without postulating any *a priori* constitutive assumption at the macro-scale. However, the major challenge is to efficiently compute the macroscopic tangent or Jacobian, if a Newton-type nonlinear solver is used, which is consistent with the evolution of the macroscopic stress at the macroscale material point. The Jacobian-free multiscale modeling technique circumvents explicit computation of the Jacobian at the macro-scale by using a Newton-Krylov process [1]. This has a major advantage in terms of storage requirements and computational cost over existing approaches based on homogenized material coefficients in which explicit Jacobian computation is required at every Newton step. A particularly interesting application of this method is being pursued in computing the mechanical response of polycrystalline aggregates of FCC metal subject to neutron irradiation with dislocation and defect density-based hardening rules that is shown to capture the experimentally observed grain- level phenomena [2].

References

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MODELLING DAMAGE DEVELOPMENT AND CRACK GROWTH IN WELDED COMPONENTS

Alan C.F. Cocks

Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ, UK, alan.cocks@eng.ox.ac.uk

Focus Material: Metals

Focus of the Presentation:

(i) Physics-based multi-scale model development;

Abstract

This paper considers the development of empirical and physical based models for damage development and crack growth in rate dependent materials. Two classes of problems are considered which involve the failure of dissimilar metal welds. The first problem concerns the creep failure of ferritic martensitic steels welded to a stainless steel or nickel based alloy. As the stress and temperature are decreased there is a transition from base metal failure to type IV cracking within the Heat Affected Zone of the ferritic steel, and then to interfacial failure. In the second problem we consider the effect of hydrogen on the fracture of a low alloy steel/nickel based alloy weld. At low hydrogen concentration the failure is ductile, but as the concentration is increased there is a transition to a quasi- cleavage mode within a narrow interface region on the Nickel side of the weld, which contains a fine distribution of M_7C_3 carbides. In this second problem rate dependence arises from the diffusion of hydrogen.

In this paper we concentrate on failures at, or close to, an interface. We describe models which take into account the details of the local (evolving) microstructure. For each problem, our models make use of cohesive or interface elements. For the creep problem the rate dependent interface elements contain information about the evolving local precipitates and cavities. We calibrate the models against micro and macro experimental data. In the case of hydrogen embrittlement we place cohesive elements around the fine precipitates, whose properties depend on the local accumulated plastic strain and hydrogen concentration.

DYNAMIC SPALLATION OF FILM/SUBSTRATE INTERFACES TAILORED WITH SELF ASSEMBLED MONOLAYERS: A MULTISCALE MODEL OF INTERFACE ROUGHNESS EFFECT

Philippe H. Geubelle¹, Chen Zhang², Jaeuk Sung³, and Nancy Sottos²

1. Aerospace Engineering, University of Illinois, geubelle@illinois.edu,
2. Aerospace Engineering, University of Illinois, czhang49@illinois.edu,
3. Materials Science and Engineering, University of Illinois, jsung12@illinois.edu,
4. Materials Science and Engineering, University of Illinois, n-sottos@illinois.edu

Focus Material: Other

Focus of the Presentation: Physics-based multi-scale model development

Abstract

Due to the flexibility that they offer in the selection of the end groups attached to the substrate and film materials, self-assembled monolayers (SAMs) composed of very short (nanometer-long) aligned polymer chains have been proposed as a unique way to tailor the electrical, thermal and mechanical properties of interfaces. In this combined experimental and computational study, we investigate the impact of the SAMs on the failure properties of a gold film/silicon substrate interface. In particular, we study SAMs with methyl (-CH₃) and mercapto (-SH) terminated functional groups, introduced along the film/substrate interface through transfer printing.

In the experimental component of the project, we adopt a non-contact laser-based spallation technique to measure the failure strength of a silicon/SAM/gold system. Results show a strong dependence of the failure strength of the interface on the choice of SAM. Detailed AFM and XPS analyses performed on the post-spallation surfaces provide information on the roughness profile and chemical composition of the failure surface.

On the modeling side, we develop a multiscale model that combines a cohesive failure model derived from MD simulations of the spallation event with a continuum model of the bending response of a film printed on a rough interface of varying wavelength and amplitude.

References

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STOCHASTIC MODELING FOR PERFORMANCE AND DESIGN ACROSS SCALES

Roger Ghanem University of Southern California
Los Angeles, CA 90089 ghanem@usc.edu

Abstract

Stochastic models entail packaging knowledge in a way that enhances its relevance to decision making. Specifics of this task clearly depend on 1) what knowledge is available, 2) which decisions are of interest, and 3) what tools are available for packaging knowledge. While decision-making undoubtedly benefits from anticipating the future, the value of the associated inference is limited by the confidence in this anticipation. A distinguishing feature of today's scientific exploration is the ability to not only observe physical phenomena at their smallest constituents, but also to resolve their behavior with mathematical models. This was enabled by technological advances in sensing and computing, and matched by advances in theoretical and computational mathematics. As a result of these developments, new perspectives have recently emerged on the substance of scientific knowledge that have critical significance to uncertainty quantification. Specifically, we are constantly faced with the need to integrate, on the one hand, streams of information associated with a hierarchy of fundamental principles (entailing causality) and on the other hand information associated with joint observations. Distinct mathematical constructs have typically been associated with these flavors of knowledge, yielding, respectively, advances in computational science and data analytics. There is a pressing need to develop rational and credible concepts and algorithms for fusing these manifestations of knowledge in a way that best articulates the value of technological developments. This talk will describe recent advances at the University of Southern California in tackling design-relevant predictions for applications where characterization of extremes is crucial notwithstanding multiscale and multiphysics effects.

UPSCALED MODELS OF RANDOM HETEROGENEOUS MATERIALS VIA PROBABILISTIC CHARACTERIZATION OF LOCAL STRUCTURE-PROPERTY RELATIONSHIPS

L.L. Graham-Brady¹, A. Tonge², and F. Huq³

1. Johns Hopkins University, Baltimore, MD, lori@jhu.edu,

2. Army Research Laboratory, Aberdeen, MD, andrew.l.tonge.ctr@mail.mil

3. Johns Hopkins University, Baltimore, MD

Focus Material: Ceramics

Focus of the Presentation: *Probabilistic modeling & uncertainty quantification*

Abstract

Failure of most brittle materials is driven by the initiation, propagation and coalescence of microcracks originating from pre-existing microstructural defects, such as grain boundaries or processing-induced pores/inclusions. Under static loading, cracks associated with the largest, most deleterious defects govern the behavior, so that Weibull statistics provide a suitable construct for identifying macro-scale strength. Under high-rate loading, however, cracks associated with a wide range of defects are mobilized; therefore, the extreme-value assumption inherent in the Weibull model is no longer valid for dynamic strength. The current work upscales a micromechanics model linking the randomly varying local defect population to the randomly varying local constitutive response. This micromechanics model serves as the basis for a constitutive model associated with the local defect population underlying individual integration points in a macro-scale analysis. Challenges arise in addressing model efficiency when tracking the crack growth of multiple families at each integration point, in incorporating coalescence of cracks, and in addressing the anisotropy of material compliance associated with preferential directions of crack growth. Results show that representation of random local variations in the constitutive behavior is key to obtaining physically reasonable results.

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