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13. ABSTRACT (Maximum 200 words)

The goal of this program was to develop incompatibility-based concepts for linking the kinematics of finite plastic deformation and failure modes across multiple length scales in crystalline and polycrystalline metallics. To do so, we consider the variation through the microstructure of thermodynamic driving forces for damage initiation and growth associated with strong lattice rotations and strain energy localization near heterogeneities such as second phase particles or grain boundary triple points. Emphasis is placed on multiple length scale modeling of plastic deformation and damage for micro-, meso- and macro-levels. Such models are novel and much more inclusive than traditional continuum models of underlying microstructural features. Contributions of entities such as cracks, voids or shear bands are treated in a consistent, multiscale manner within this kinematical framework. We combine the work on fundamentally new decompositions of the finite deformation gradient for plasticity and damage with computational simulations and measurement of sub-grain scale stretch and rotation fields to validate and understand implications. Experiments are performed on both polycrystalline pure copper as well as copper doped with antimony to promote intergranular fracture. Novel methods of measurement down to scale of 5-10 microns are developed for curved specimens using lithographic grids.

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Final Project Report – ARO DAAD19-99-1-0221: 5/99-5/03
Evolving Multiscale Deformation and Damage in Polycrystals
August 12, 2003

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Research Objectives

The goal of this program was to develop incompatibility-based concepts for linking plastic deformation and failure modes across length scales in metals, taking into account effects of material microstructure in a more intimate way than existing, state-of-the-art temperature dependent viscoplasticity and damage mechanics relations. In so doing, we consider variation through the microstructure of driving forces for damage initiation and growth associated with strong lattice rotations near heterogeneities such as second phase particles or grain boundaries. Emphasis is placed on multiple length scale models for micro, meso and macro levels for inelastic deformation and damage within heterogeneous, polycrystalline microstructures. Such models are potentially useful in practical applications involving large deformation at high rates of strain such as penetration, blast wave propagation, machining, etc.

Approach

We have pursued a combined strategy of developing new analytical principles for averaging deformation and damage effects at finite strain in polycrystalline metals, and have implemented these methods in computational mechanics (finite element method) to analyze incompatibility fields in polycrystalline materials subjected to large strain plastic deformation. The analysis of deformation has been combined with distributed cohesive fracture along grain boundaries. Furthermore, innovative experiments have been developed by extending photolithographic techniques from microelectronics and MEMS to measure subgrain deformation fields in Cu polycrystals with average grain size below 100 microns, enabling comparison with our models for microstructure-scale behavior. Experiments have been conducted on Cu polycrystals with and without trace Antimony, a potent grain boundary segregant that promotes intergranular fracture, enabling comparison with models and effects of computed incompatibility fields characterized by local plasticity and fracture.

Significance – Army Value

In addition to their fundamental contribution to a new method of decomposing elastic and plastic finite deformation in heterogeneous elastic-plastic materials, it is expected that these results will have an impact on the level of *incorporation of microstructure information* in future calculations evaluating concepts for armor/anti-armor and for applications such as advanced penetrator concepts that rely on texture control, optimizing resistance to break-up of shaped charge jets, impact behavior for hypovelocity and hypervelocity projectiles, and manufacturing and dual use technology for large strain problems (machining, metal forming, etc.). Polycrystal plasticity theory is prohibitively intensive for large scale calculations and also may not address all relevant physical aspects of transition from behavior of single grain to polycrystal – we need mesoscopic/macroscopic approaches that combine attributes of micro/mesoscopic theories based on limited but highly detailed, sophisticated material representations with macroscale descriptions. Current use of critical effective strain as a failure criterion, sometimes augmented by the notion of internal porosity, is not descriptive enough to reflect effects of varying microstructure. This work has contributed to a multiscale modeling constitutive modeling framework that (i) reflects microstructure heterogeneity at lower length scales in the kinematical relations and (ii) explores novel failure criteria based on the incompatibility field strengths that arise from this heterogeneity field (i.e., incompatibility fraction and shift criteria).

Accomplishments

Both general scientific advances as well as Army application-specific advances have been made in this program, with additional support of an AASERT grant that supported students involved in this work directly (AASERT: ARO DAAG55981021). Multiscale modeling is a current prominent theme of interest to many agencies. Comparison of the computational and experimental results has led to improved understanding of collective mesoscopic combined deformation and damage behaviors at large strain. Improved continuum concepts have been developed to interpret computational analyses conducted over statistical volumes of grains in terms of (i) a new decomposition of the deformation gradient in a granular medium with eigenstrains deriving from diffuse or localized dislocation plasticity, voids, and intergranular damage, and (ii) new failure criteria based on incompatibility measures and attendant accommodation measures that reflect mechanisms more precisely than existing mesoscopic or macroscopic failure laws. More directly applicable to the types of penetrator analyses conducted by the Army Research Laboratory, we have coupled polycrystal plasticity models with typical macroscopic ISV models that are easy to use and to fit model parameters with experimental results, with different methods for incorporating evolution of crystallographic texture (so-called multiscale crystal plasticity models). This effort has also resulted in the development of faster algorithms for numerical integration of rate independent crystal plasticity theory and approximations for moderately rate dependent models. We have also followed new directions in using interface separation elements with crystal plasticity for polycrystal plasticity calculations for ensembles of grains, averaging results in our new framework, and comparing to experiments for Cu and Cu doped with Sb (Antimony), which serves to selectively produce grain boundary fracture. Finally, limited molecular dynamics simulations of interface separation in Cu-Cu bicrystals with various misorientations have allowed us to draw implications necessary to develop preliminary forms for history and loading mode mixity-dependent cohesive fracture potentials for grain boundaries.

Technology Transfer

We have interacted closely with the mechanics of materials group at Sandia National Laboratories in Livermore, California (D.J. Bammann, M.F. Horstemeyer, J. Zimmerman and D.A. Hughes) with the goal of developing local and nonlocal internal state variable models and practical user methodologies for parameter estimation to address large strain deformation and failure of polycrystalline metals for applications ranging from welding to phase transformations to dynamic impact. We are presently collaborating with Dr. Bammann on coupling his work on nonlocal theory of subgrain dislocation interactions with our polycrystalline homogenization effort. We have also actively interacted with Dr. Scott Schoenfeld of the U.S. Army Research Laboratory regarding rate- and temperature-history constitutive relations, polycrystal plasticity integration algorithms and hybrid schemes for textured penetrators and EFPs (former PhD student Bob McGinty spent time at ARL with Dr. Schoenfeld and worked on cooperative problems involving stability of shaped charge jets). Finally, recent PhD graduate John Clayton is presently a post doctoral research fellow at ARL in Aberdeen.

Publications

Related Refereed Journal Articles Published

1. McDowell, D.L., "Modeling and Experiments in Plasticity," special volume on Research Directions in Solid Mechanics, Ed. G.J. Dvorak, Int. Journal of Solids and Structures, Vol. 37, 2000, pp. 293-309 (invited).
2. McDowell, D.L., "Materials Design: A Useful Research Focus for Inelastic Behavior of Structural Metals," Special Issue of the Journal of Theoretical and Applied Fracture Mechanics, Prospects of Mesomechanics in the 21st Century: Current Thinking on Multiscale Mechanics Problems, eds. G.C. Sih and V.E. Panin, Vol. 37, 2001, pp. 245-259 (invited).
3. Butler, G.C., Stock, S.R., McGinty, R.D. and McDowell, D.L., "X-Ray Microbeam Laue Pattern Studies of the Spreading of Orientation in OFHC Copper at Large Strains," ASME Journal of Engineering Materials and Technology, Special Issue on Micromechanics, Vol. 124, 2002, pp. 48-54.
4. Clayton, J., Schroeter, B., Graham, S. and McDowell, D.L., "Distributions of Stretch and Rotation in Polycrystalline OFHC Cu," ASME Journal of Engineering Materials and Technology, Vol. 124, No. 3, 2002, pp. 302-313.
5. Zhou, M. and McDowell, D.L., "Equivalent Continuum for Dynamically Deforming Atomistic Particle Systems," Phil. Mag. A, Vo. 82, No. 13, 2002, pp. 2547-2574.
6. Clayton, J.D. and McDowell, D.L., "A Multiscale Multiplicative Decomposition for Elastoplasticity of Polycrystals," International Journal of Plasticity, Vol. 19, No. 9, 2003, pp. 1401-1444.
7. Schroeter, B.M. and McDowell, D.L., "Measurement of Deformation Fields in Polycrystalline OFHC Copper," International Journal of Plasticity, Vol. 19, No. 9, 2003, pp. 1355-1376.
8. Clayton, J.D. and McDowell, D.L., "Finite Polycrystalline Elastoplasticity and Damage: Multiscale Kinematics," International Journal of Solids and Structures, accepted for publication, June 2003.
9. Clayton, J.D., Bammann, D.J. and McDowell, D.L, "Anholonomic Configuration Spaces and Metric Tensors in Finite Elastoplasticity," submitted to International Journal of Nonlinear Mechanics, December 2002, accepted.

Related Submitted Journal Articles

1. McGinty, R.D. and McDowell, D.L., "Application of Multiscale Crystal Plasticity Models to Forming Limit Diagrams," Submitted to ASME Journal of Engineering Materials and Technology, October 2002.
2. Clayton, J.D., McDowell, D.L. and Bammann, D.J., "A Geometric Description o the Kinematics of Crystal Defects," submitted to Applied Mechanics Reviews, November 2002.
3. Spearot, D.E., Jacob, K.I. and McDowell, D.L., "Nonlocal Separation Constitutive Laws for Interfaces and their Relation to Nano-scale Simulations," submitted to Mechanics of Materials, December 2002.

4. Clayton, J.D., Bammann, D.J. and McDowell, D.L, "A Multiscale Gradient Theory for Single Crystalline Elastoviscoplasticity," submitted to International Journal of Engineering Science, December 2002.
5. Clayton, J.D. and McDowell, D.L., "Homogenized Finite Elastoplasticity and Damage: Theory and Computations," submitted to Mechanics of Materials, March 2003.

Conference Proceedings/Presentations/Seminars

1. Butler, G.C., Stock, S.R., McGinty, R.D. and McDowell, D.L., "X-Ray Microbeam Diffraction Studies of Large Strain Dislocation Substructure Formation in OFHC Copper," Proc. AEPA 2000, *Advances in Engineering Plasticity*, Hong Kong, June 12-16, 2000, Trans Tech Publ., Ltd, Switzerland, pp. 165-170.
2. Butler, G.C., McGinty, R.D., and McDowell, D.L., "An Internal State Variable Model for Dislocation Substructure Formation in Polycrystal Plasticity," ICTAM 2000, Chicago, IL, August 29, 2000. (presentation only)
3. Spearot, D.E., Jacob, K.I., Zhou, M. and McDowell, D.L., "Nonlocal Separation Constitutive Laws for Interfaces and their Relation to Nanoscale Simulations," 1st Georgia Tech Conference on Nanoscience and Nanotechnology, October 16-18, 2000, Atlanta, GA. (presentation only)
4. McGinty, R.D. and McDowell, D.L., "Multiscale Modeling Concepts for Finite Deformation of Polycrystalline Metals," in *Continuous Damage and Fracture*, Elsevier, Cachan, France, October 23-27, 2000, pp. 29-39.
5. Schroeter, B., Clayton, J., Graham, S., and McDowell, D.L., "Distributions of Stretch and Rotation in Polycrystalline OFHC Cu, summer ASME/ASCE/SES Applied Mechanics meeting, San Diego, CA, June 27, 2001. (presentation only)
6. McDowell, D.L., "Experimental Evidence of Length Scale Effects," Workshop on Nonlocal Effects in Solid Mechanics, Sandia National Laboratories, Livermore, CA, July 9, 2001. (presentation only)
7. McDowell, D.L., "Internal State Variable Models and Length Scales," Workshop on Nonlocal Effects in Solid Mechanics, Sandia National Laboratories, Livermore, CA, July 9, 2001. (presentation only)
8. McDowell, D.L., "Self-Organization Aspects of Nonlocal Field Models," Workshop on Nonlocal Effects in Solid Mechanics, Sandia National Laboratories, Livermore, CA, July 10, 2001. (presentation only)
9. McDowell, D.L., "Some Mechanics Needs in Modeling Nanoscale Phenomena," ARO Workshop on Nanoscale Mechanics, Panama City, FL, April 9, 2002. (presentation only)
10. McDowell, D.L., "Homogenization Concepts for Granular and Particle Systems," Conference in Mechanics of Material, invited participant, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, Germany, May 5-11, 2002. (presentation only)
11. Clayton, J.D. and McDowell, D.L., "A Multiscale Multiplicative Decomposition for Elastoplasticity of Polycrystals," Proc. Plasticity '02, The 9th Int. Symp. on Plasticity and its Current Applications, Plasticity, Damage and Fracture at Macro, Micro and Nano Scales, eds. A.S. Khan and O. Lopez-Pamies, NEAT Press, 2002, pp. 696-698.
12. Clayton, J.D. and McDowell, D.L., "A Multiscale Model for Deformation and Failure of Polycrystals", Mesomechanics 2002, ed. R. Pyrz, Aalborg University, Aalborg, Denmark, August 26-30, 2002.

13. McDowell, D.L., "Dan Drucker's Legacy: Ockham's Razor and Plasticity Theory," Dr. Daniel C. Drucker Memorial Symposium, University of Florida, Gainesville, FL, Oct. 8-10, 2002. (invited presentation)
14. Clayton, J.D., Bammann, D.J. and McDowell, D.L., "A Multiscale Gradient Theory for Elastoviscoplasticity of Single Crystals," Proc. SES 2002, Penn State University, State College, PA, Oct. 13-16, 2002.
15. Spearot, D., Jacob, K.I. and McDowell, D.L., "Nonlocal Separation Constitutive Laws for Interfaces Informed by Nano-Scale Simulations," SES 2002, Penn State University, State College, PA, Oct. 13-16, 2002.
16. Clayton, J.D., McDowell, D.L. and Bammann, D.J., "A Multiscale Gradient Model of Finite Crystalline Elastoviscoplasticity," Proc. 16th U.S. Army Symposium on Solid Mechanics, Charleston, SC, May 4-7, 2003.
17. Clayton, J.D., McDowell, D.L. and Bammann, D.J., "Modeling Dislocations and Disclinations with Finite Micropolar Elastoplasticity," Proc. *Plasticity 2003*, Quebec City, Canada, July 7-12, 2003.

PhD Theses Completed:

1. Robert D. McGinty (AASERT), "Multiscale Representation of Polycrystalline Inelasticity," August 2001; presently at Mercer College, Macon, GA
2. John D. Clayton, "Homogenization and Incompatibility Fields in Finite Strain Plasticity," December 2002; presently post doc at ARL

MS Theses Completed:

1. Brian.M. Schroeter, "Techniques for Micro- and Meso- Scale Measurements of Rotation and Stretch Processes in Metallic Polycrystals," May 2001.
2. Douglas Spearot, "Interface Separation Laws based on Atomistics," May 2002.
3. Jean-Baptiste Bergugnat, "Strain and Lattice Rotation Fields of Deformed Polycrystals," December 2002.

Honors & Awards: D.L. McDowell

- Georgia Tech Outstanding Doctoral Thesis Advisor Award, 2000, in recognition of the achievements of a faculty member's doctoral students who completed all degree requirements from January 1, 1995 to December 31, 1999.
- American Foundrymen's Society Team Award, USAMP-AMD-DPO Project, 1995-2000.
- Elected as a member of the Board of Directors, Society of Engineering Science (SES), 2000-2003.
- Elected as a member of the M&IE Alumni Board for 1999-2002, Dept. of Mechanical and Industrial Engineering, University of Illinois at Urbana-Champaign.
- Vice President, Society of Engineering Science (SES), 2001
- President of SES, 2002
- <u>Microstructure-Property Model Software</u> Selected by R&D Magazine as One of the 100 Most Technologically Significant New Products of the Year (2000), with contributions in my role as consultant to prime developer Sandia National Laboratories (DOE), through joint collaboration with the following team: D. Bammann, M. Callabresi, M. Chiesa, M. Horstemeyer, G. Johnson (UC-Berkeley),

J. Lathrop, M. Lusk (Colorado School of Mines), E. Marin, D.McDowell (Georgia Tech), V. Prantil, R. Regueiro and P. Taylor.

- Georgia Tech Outstanding Interdisciplinary Activities Award, 2001, in recognition of the achievements of a faculty member to engage in a range of interdisciplinary research and educational activities.
- ASTM Committee E.08 Award of Appreciation for outstanding service as the ASTM Representative on the U.S. National Committee on Theoretical and Applied Mechanics, 1994-2001, November 2001.
- SAIC Student Guidance Award for the paper "Crack Plane Influence on Non-Linear and Time-Dependent Fracture of Bimaterials" by PhD advisee Ali Page Gordon, 2001.
- ASTM Annual Fatigue Lecturer, Miami Beach, FL, Nov. 5, 2002.