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.
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 hypervelocity 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

Related Submitted Journal Articles


Conference Proceedings/Presentations/Seminars


PhD Theses Completed:

MS Theses Completed:

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 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
- Microstructure-Property Model Software 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 Annual Fatigue Lecturer, Miami Beach, FL, Nov. 5, 2002.