US Army Research Laboratory Materials Center of Excellence


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under contract W911NF-06-2-0006

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This cooperative research program emphasizes collaborative research between The Johns Hopkins University and the US Army Research Laboratory toward well-defined common goals: the understanding and development of advanced lightweight materials for vehicular protection, focusing on high-strain-rate/high-stress testing, determining the operative deformation and failure mechanisms, and developing relevant models to allow for materials design. This report summarizes the research carried out during 1 July 2010 through 30 June 2011 in the following areas: 1) nanomicro aluminum research thrust, 2) nanostructured magnesium research thrust, 3) dynamic failure and damage mechanisms research thrust, 4) modeling of body-centered-cubic nanostructures research thrust, 5) high-rate loading of piezoelectric ceramics research thrust, 6) administration, education, training, and collaborative structures, and 7) list of theses, publications, and presentations from the various thrust areas.
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1. Introduction

This cooperative research program emphasizes collaborative research between The Johns Hopkins University and the US Army Research Laboratory (ARL) toward well-defined common goals: the understanding and development of advanced lightweight materials for vehicular protection. The Johns Hopkins side of the collaboration is operated through a science-driven, problem-directed center: the Center for Advanced Metal and Ceramic Systems (CAMCS). The research thrusts and the collaborative structures of the Center provide a basis for the substantial enhancement and continuous improvement of the scientific and technical capabilities of ARL, and particularly of the Weapons and Materials Research Directorate.

This document is an annual report for research performed in the last 6 months of the calendar year 2010 and the first 6 months of the calendar year 2011. Each research thrust operates a Collaborative Research Group, or CRG, with joint responsibility for the development of the research. The next few pages present individual reports for each research thrust during the period indicated above. Where revised objectives are presented, these have been discussed and approved by the CRG unless otherwise indicated. Note also that the ARL collaborators listed represent all individuals who have indicated a desire to be involved in each thrust.
2. **Nanomicro Aluminum Research Thrust**

Core Faculty: KT Ramesh, KJ Hemker


Graduate Student: Emily Huskins

### 2.1 Long-Range Objectives

The long-range objectives of this study are as follows:

- Determine the deformation and failure mechanisms in nanomicro aluminum (Al) alloys and their composites subjected to impact rates of loading.
- Develop models for the dynamic deformation and dynamic failure of nanomicro composites, with the objective of enabling materials design.

### 2.2 Objectives for July 1, 2010, to June 30, 2011

**Third Quarter 2010:**
- Continue to develop model for thermal softening of nanomicro Al (and more generally) metals; tie to experimental data and trimodal data.

**Fourth Quarter 2010:**
- Expand model to include microstructural stability of nanocrystalline and nanomicro Al alloys at high rates and high temperatures.

**First Quarter 2011:**
- Complete high-strain-rate thermal softening model for nanocrystalline and ultra-fine-grained (UFG) aluminum-based materials.

**Second Quarter 2011:**
- Determine implications of 2139 Al model developed in 2010 on potential for strengthening the material.
- Complete doctoral thesis (Huskins).

### 2.3 Research Summary

High-temperature, high-strain-rate compression experiments were conducted on an UFG Al-1100 processed by equal channel angular pressing through 8 passes of
route B (provided by Suveen Mathaudhu). The temperature range examined was 298–573 K. It was found that the minute-long preheating procedure resulted in significant recovery and grain growth for this material. As a consequence, the initial grain size of the material varies with the testing temperature (i.e., the final preheating temperature). The temperature-dependent mechanical response is thus determined by testing samples, which have experienced the same preheating conditions, at both room temperature (after the sample is quenched) and the preheating temperature (immediately after desired temperature is reached). This ensures the initial microstructure (e.g., grain size and dislocation density) is the same for both tests. Fig. 2.1 shows stress-strain curves for 2 testing temperatures: 473 and 573 K, both tested at 6000 s⁻¹. The dashed lines represent room temperature tests, while the solid lines represent high-temperature tests. The colors correspond to preheating temperature (labeled as PH). The black curve is the as-received material tested at room temperature and 6000 s⁻¹ for comparison. For both preheating temperatures, the room temperature tests show lower flow stress and higher strain hardening than the as-received material. This is a result of both recovery and grain growth during preheating.

![Stress-strain curves for Al-1100 preheated to 473 and 573 K tested at room temperature and their respective preheating temperature at 6000 s⁻¹. Results for the as-received material are included for comparison.](image)

Samples preheated and tested at high temperatures show both a decrease in flow stress and a decrease in strain hardening as compared to the room temperature response. From this we conclude that 2 thermal activation mechanisms are occurring during high-temperature deformation:
1) An increase in dislocation mobility

2) A decrease in dislocation density through annihilation due to cross-slip

Future work will be conducted using transmission electron microscopy micrographs to determine grain size evolution related to preheating temperature. We will also investigate any post-deformation microstructural changes.

In addition, a physically based constitutive model is being developed for nanomicro Al materials. The mechanisms that are accounted for in the model include the following:

- Temperature, strain rate, and grain size effects
- Evolution of dislocation density during deformation
- Evolution of grain size during deformation

The model is a modified Kocks-Mecking model, where the internal variable (dislocation density) evolves during deformation. The evolution equation is of the following form:

\[
\frac{d\rho}{d\varepsilon^p} = \left( \frac{d\rho}{d\varepsilon^p} \right)^+ - \left( \frac{d\rho}{d\varepsilon^p} \right)^- = M \left( \frac{\alpha \sqrt{\rho}}{b} + \frac{\beta}{bd} \right) - M \left( C \rho s_k(\varepsilon, T) \right),
\]

where \( \rho \) is the dislocation density, \( \varepsilon^p \) is the plastic strain, \( M \) is a Taylor factor, \( b \) is the Burgers vector, \( d \) is the grain size, \( \alpha, \beta \) are constants, \( C \) is a grain size–dependent term, and \( s_k \) is a rate- and temperature-dependent function of the Arrhenius form. The first term on the right in Eq. 1 is a dislocation “source” term, in which an increase in dislocation density occurs through accumulation of both statistically stored and geometrically necessary dislocations. This term is grain size dependent through the geometrically necessary dislocations and is related to Stage II hardening. The second term on the right is a dislocation “annihilation” term, in which a decrease in dislocation density is due to thermally activated cross-slip. This term is considered to be grain size dependent through parameter \( C \) and is related to Stage II hardening.

Further work will include a grain-size evolution equation, which can be used within the internal variable evolution equation. Model parameters are currently being obtained from literature data on commercially pure and high-purity Al.
2.4 Collaborative Interactions

We are collaborating with Profs J Schoenung and E Lavernia of UC Davis on Al-5083-based nanomicro materials.

2.5 Publications and Presentations


3. **Nanostructured Magnesium Research Thrust**

Core Faculty: KT Ramesh


Postdoctoral Fellow: Partial support of postdoc TBD

### 3.1 Long-Range Objectives

The long-range objectives of this study are as follows:

- Determine the potential of nanostructured magnesium (Mg) alloys for vehicle applications.
- Examine the issues of formability and corrosion resistance of nanostructured magnesium alloys and their composites.

### 3.2 Objectives for July 1, 2010, to June 30, 2011

**Third Quarter 2010:**

- Analysis to determine the stored defects and the functioning mechanisms in selected single-phase ultra-fine-grained (UFG) (<1 μm) Mg alloys
  - Is twinning suppressed in UFG?
  - Dislocation storage for work hardening?

**Fourth Quarter 2010:**

- Determine mechanisms in selected single-phase UFG Mg at high strain rates through transmission electron microscopy (TEM), molecular dynamics, and modeling.

**First Quarter 2011:**

- High-strain-rate evaluation (Kolsky bar rates) of ball-milled Mg produced by Darling et al.

**Second Quarter 2011:**

- High-strain-rate evaluation (Kolsky bar rates) of UFG and nanocrystalline Mg produced by the US Army Research Laboratory (ARL) and other collaborators.
3.3 Research Summary

A series of experiments at high strain rates have been carried out to investigate the mechanical properties of UFG AZ31B Mg alloys (Fig. 3.1) processed by equal channel angular extrusion. TEM has been performed to study the microstructures of the samples before and after testing. These results show that, when the grain size is reduced down to submicrons, the Hall-Petch relationship may no longer hold.

We are awaiting supply of ball-milled magnesium from our ARL collaborators.

![Grain structure and yield strength graph](image)

Fig. 3.1 (Left) Grain structure of the ultra-fine-grained (UFG) AZ31B Mg alloy processed by equal channel angular extrusion. The grain size is about 250 nm. (Right) The yield strength of the UFG material no longer follows the Hall-Petch relationship.

3.4 Collaborative Interactions

We continue to collaborate with Suveen Mathaudhu and Bob Dowding.

3.5 Publications and Presentations


5. Li B, et al. Twinning without a twinning plane. TMS; 2011; San Diego, CA.
4. **Dynamic Failure and Damage Mechanisms Research Thrust**

Core Faculty: KT Ramesh, L Graham-Brady, K Hemker


Postdoctoral Research Fellow: Dr Nitin Daphalapurkar

Graduate Student: Cindy Byer

ARL Graduate Student: Cyril Williams

4.1 **Long-Range Objectives**

The long-range objectives of this study are as follows:

- Characterize micromechanisms of dynamic deformation and failure developed within the other Center for Advanced Metal and Ceramic Systems thrusts.

- Develop physics-based models for the massive failure of lightweight metallic systems.

- Develop mechanism-based models for the evolution of damage within heterogeneous materials under dynamic loading.

4.2 **Objectives for July 1, 2010, to June 30, 2011**

Third Quarter 2010:

- Modeling for size effects in magnesium (Mg).

- Continue development of twinning model for face-centered cubic (FCC) nanomaterials, with applications to the trimodal and other systems.

Fourth Quarter 2010:

- Begin development of mechanism-based multiscale approach to microstructure design as part of longer-term thrust.

First Quarter 2011:

- Continue development of mechanism-based multiscale approach to microstructure design for dynamic applications.

- Understand size effects in magnesium vis-à-vis etching and orientation.
• Conduct shock recovery experiments on 1100 aluminum (Al).

Second Quarter 2011:
• Continue development of mechanism-based multiscale approach to microstructure design for dynamic applications.
• Use in situ testing technique (with help from Schuster) to examine size effects and twinning mechanisms in Mg.
• Investigate the effects of microstructural evolution on the spall response of 1100 Al.

4.3 Research Summary

4.3.1 Mechanism-Based Multiscale Approach to Microstructural Design for Dynamic Applications

Plastic deformation in certain nanocrystalline metals (grain sizes <100 nm) or under certain conditions is associated with profuse activation of partial dislocations with grain boundaries acting as both the source and the sink. An understanding of the homogeneous nucleation of dislocations is a necessary prerequisite for the understanding of a number of fundamental problems in plasticity, including the onset of dislocation development during nanoindentation, the development of plasticity in nanoscale domains within which heterogeneous sources may be difficult to find, the provision of fundamental information to discrete dislocation dynamics simulations in source-limited domains, and the development of criteria for the relative roles of dislocation nucleation and dislocation multiplication.

We use molecular dynamics (MD) simulations of pure Al to investigate the orientation dependence of deformation mechanisms and show that 2 types of twins can be generated. Theoretical calculations are used to understand the effect of loading orientation on the activation of twins. The theoretical framework incorporates 1) a tensorial stress state, 2) dislocation loops, and 3) nonsingular core energies for accurate descriptions of criteria for partial dislocation activation. Both the theoretical predictions and the MD simulation demonstrate that twins should be possible (but rare) in nanocrystalline aluminum. We examined, in particular, the mechanism of twinning through co-operative activation of partial dislocations on the basis of theoretical considerations and support these results through MD simulations.
4.3.1.1 Molecular Dynamics Simulation Results

The specific shearing orientations (Fig. 4.1) that we have chosen to examine provide a full sampling of the entire orientation space, given the crystal symmetry. Within the subspace that we have examined, extended twins are observed for shearing along OA, extended dislocations are observed for shearing (thick arrow) along OC, and very limited twinning followed by dislocation motion is observed for shearing along OE. The intermediate orientations represent mixtures of these deformation modes. Examining the full orientation space, therefore, one observes that dislocation slip is the dominant mechanism that is activated in most of the orientation space, with small subregions within which the twinning mechanism is preferentially activated, and an even smaller region where extended twins may be activated.

![Orientation space under consideration, 0 ≤ θ ≤ 600°](image)

4.3.1.1 Theoretical Calculations

The shearing deformations considered in this work make it possible to explore the oriented loading space and observe the resulting deformation mechanisms (full dislocations; extended dislocations; leading, trailing, and twinning partials; and subsequent twinning through multiple mechanisms) under constrained volume conditions. Existing results in the literature have suggested that slip and twinning may act as competing mechanisms to each other. Our MD simulations results are consistent with this view but also demonstrate the importance of loading orientation and the potential richness of phenomena that can be activated even in high-stacking fault energy materials like Al. This is important in problems such as the dynamic deformation of nanocrystalline Al where high stresses may be sustained in any case. In the next section, we consider the potential mechanisms that can develop in this system from a theoretical viewpoint and seek to understand the likelihood of observing these phenomena.
We consider the stresses needed to propagate a leading partial dislocation loop and then examine the stresses needed to develop 2 competing mechanisms, either a trailing partial dislocation on the same glide plane leading to the development of an extended dislocation (slip) or a successive subsequent propagation of a twinning partial dislocation on the adjacent glide plane leading to the development of a deformation twin. In both cases we assume that a leading partial dislocation loop has already been activated. In each case we consider the entire range of loading orientations and thereby develop a sense of the relative ease of activation of the dislocation slip and twinning mechanisms in each orientation. The following simple theoretical analysis does not account for the inertial terms associated with the dislocation motion. We seek to understand the likelihood of twinning in Al by examining the relative ease with which these 2 mechanisms are activated.

Our results (Fig. 4.2) show that for most of the orientation space within a single crystal subjected to shearing deformations, it is favorable to activate a trailing partial immediately after the leading partial dislocation has been activated, leading to the traditional dislocation slip mechanism, with generally small stacking fault widths. For a very small range of orientations (0 ≤ θ ≤ 10 from the leading partial Burgers vector), it appears to be easier to activate a twinning partial dislocation leading to a twin. However, the orientation space available for twinning in the case of Al is much smaller compared to that available for slip. This indicates that it should be difficult, but not impossible, to find twins in Al.

![Fig. 4.2 Orientation-dependent activation stress for a trailing and twinning partial dislocation](image)

**4.3.2 Micromechanical Testing of Hexagonal Close-Packed Crystals**

The size effects and orientation dependence of deformation mechanisms associated with single crystals under uniaxial compression are becoming an increasingly popular area of study. Despite the growing collection of microcompression literature that shows for some materials, decreasing the
diameters of these microscale pillars increases the yield stresses and strain hardening rates, many questions remain, especially for hexagonal close-packed materials. In this study, we focus on the impact of initial dislocation density on deformation mechanisms and size effects in single crystal Mg. To do this, we start with 2 single crystals that are the same orientation, [0001]. The first is mechanically polished, which introduces plasticity, and therefore dislocations, to the microstructure. Thus, these micropillars have a high initial dislocation density. The second crystal is also mechanically polished; however, it is then chemically etched using a nitric acid solution. This removes part of the damaged layer introduced by mechanically polishing, lowering the initial dislocation density. Transmission electron microscopy was conducted to quantify the initial dislocation densities. These results are in Fig. 4.3 and show $\rho_{O,\text{unetched}} \approx 1.0 \times 10^{14} \text{m}^{-2}$ and $\rho_{O,\text{etched}} = 4.7 \times 10^{13} \text{m}^{-2}$, giving a difference of approximately a factor of 2.

![Fig. 4.3 Transmission electron microscopy results showing initial dislocation densities for two [0001] single crystals](image)

Microcompression experiments are conducted on micropillars (1 to 10 µm in diameter) fabricated using focused ion beam milling on both the chemically etched and unetched samples. Specimens are loaded along the [0001] c-axis and reveal that etched samples with lower initial dislocation densities exhibit a much stronger size effect than the unetched case. The response is also more stochastic in the etched sample, as opposed to in the unetched experiments. Before- and after-deformation scanning electron micrographs can be seen in Fig. 4.4. This specific specimen was etched; however, the same deformation mode (basal slip) was observed in both cases. The corresponding stress-strain curves are presented in Fig. 4.5.
We also investigated the effect of anisotropy in microcompression experiments. A single crystal oriented along [2 -3 1 4] was etched and loaded in uniaxial compression. Postmortem analysis indicates the mode of deformation was likely also basal slip, as this orientation makes an angle of 51° with the c-axis. The images taken with a scanning electron microscope can be viewed in Fig. 4.6. The stress-strain curves can be viewed in Fig. 4.7. A size effect is also observed, and the responses are stochastic, resembling the trends we saw in the etched case for compression along the c-axis. However, note the much lower stress measures for this orientation, which is expected because of the increased resolved shear stress on the basal planes.
Fig. 4.6 Before and after deformation images of a 3-µm micropillar compressed along [2 -3 1 4]

Fig. 4.7 Stress-strain curves for microcompression experiments along [2 -3 1 4]

4.3.3 Effects of Microstructural Evolution on the Spall Response of 1100 Aluminum

During severe plastic deformation of FCC metals, the material’s microstructure can evolve between 2 extremes. For example, in the case of Al, the dominant microstructure at 30% cold-rolled condition is a mixture of cells, cell blocks, dense dislocation walls, and microbands. Whilst at 80% cold-rolled condition, the microstructure is dominated by a lamellae structure. However, no in-depth study on the effects of microstructural evolution on the spall response of FCC materials has been conducted. Therefore, in this investigation the primary goal was to study the effects of microstructural evolution on the spall response of 1100 Al. The 1100 Al was cold rolled to 30% (low to moderate strains), 70% (intermediate
strains), and 80% (large strains) to achieve the desired microstructure. Shown in Fig. 4.8 is an Electron Back Scatter Diffraction micrograph of the grain structure and orientation map showing the microstructural evolution of 1100 Al under various cold-rolled conditions. The 1100-O grain structure when cold rolled to 80% is highly elongated to a lamellae structure, which is highly textured (anisotropic). Also, the low-angle grain boundaries (yellow lines in Fig. 4.8) are largely increased between 1100-O and 80% cold-rolled condition. Furthermore, the grains were observed to rotate between various cold-rolled conditions in order to accommodate the large plastic deformation.

The effects of peak pressure on all 4 conditions (O-temper, 30%, 70%, and 80% cold rolled) were studied, and the results are presented in Fig. 4.9. Please note that the pullback velocity is reported in Fig. 4.9 because it is a direct measure during the plate impact experiments. However, the spall strength is sometimes reported in the open literature. Between 4.0 and 8.5 GPa, shock hardening was found to be the dominant mechanism for the as received 1100-O Al, possibly due to large increase in dislocation density. Beyond 8.5 GPa, shock annealing was found to be the dominant mechanism possibly due to dynamic recovery because of the increase in temperature with the increase in shock pressure. However, for the 30% cold-rolled condition, shock hardening was found to be the dominant mechanism throughout the shock pressure range investigated (4–12 GPa). No change was observed for the 70% cold-rolled condition between 4 and 11 GPa. This is possibly due to dislocation saturation during the rolling process; therefore, no more dislocation can be infused into the substructure during the shock-loading process. The response of the 80% cold-rolled condition did not show any definitive trend because the pullback velocity varies widely between 4 and 11 GPa. The wide variation is possibly due to the variation in the texture from specimen to specimen. More spall experiments are planned to further investigate

![Fig. 4.8 Electron Back Scatter Diffraction grain structure and orientation map showing the microstructural evolution of 1100 aluminum under various cold-rolled conditions](image)
the variability in the pullback signal for the 80% cold-rolled condition. Soft shock recovery experiments and microstructural analysis are also planned to validate the aforementioned hypothesis for all conditions.

![Graph of pullback velocity vs. peak stress](image)

**Fig. 4.9** The effects of peak stress on the spall response of 1100 aluminum (O-temper, 30%, 70%, and 80% cold rolled)

### 4.4 Collaborative Interactions

- Dr Nitin Daphalapurkar (JHU) and Dr Brandon McWilliams (ARL), concerning mechanism-based multiscale approach to microstructure design for dynamic applications.
- Cindy Byer (JHU) and Dr Brian Schuster (ARL), concerning microscale tension and compression testing techniques and data analysis.
- Cyril Williams (ARL/JHU) and Dr Datta Dandekar (ARL Fellow), concerning shock physics and soft shock recovery experiments.

### 4.5 Publications and Presentations


4. Daphalapurkar NP, Ramesh KT. Partial dislocations and deformation twinning in pure face-centered cubic metals. Conference presentation. MS&T; Houston, TX; 2010 Oct.

5. Daphalapurkar NP, Ramesh KT. Partial dislocation nucleation and twinning in aluminum. TMS Annual Meeting and Exhibition; San Diego, CA; 2011 Mar.


5. Modeling of Body-Centered Cubic Nanostructures

Core Faculty: KT Ramesh
ARL Collaborators: Eric Klier, Brady Butler, Rich Haber, Brian Schuster
Postdoctoral Fellow: Dr Swapnil Patil

5.1 Long-Range Objectives

The focus is on the mesoscale modeling of body-centered cubic (BCC) nanomaterials with nanomicro microstructures. The global objective is to provide guidelines for microstructural design to optimize the mechanical properties and to control the failure, with the emphasis on those properties and processes that are unique to BCC materials. The approach is to use mesoscale and crystal plasticity simulations to understand deformation and failure processes.

5.2 Objectives for July 1, 2010, to June 30, 2011

Third Quarter 2010:
- Review literature on atomistic simulation of screw dislocation core in BCC crystals and understand the role of non-Schmid shear stresses on critical resolved shear stress.
- Develop crystal plasticity constitutive model for BCC single crystals, based on thermally activated motion of screw dislocations and atomistically informed non-Schmid effects.

Fourth Quarter 2010:
- Develop numerical implementation of the constitutive model in a finite-element program Abaqus by writing user subroutine UEL.
- Complete code testing and apply the model to molybdenum single crystal to determine required material properties.

First Quarter 2011:
- Implement higher-order strain gradient crystal plasticity formulation to introduce material length-scale parameters in the model to capture the size effects in BCC metals.
Second Quarter 2011:

- Develop an approach to generate specialized finite element mesh for polycrystalline template microstructure to implement grain boundary microscopic boundary conditions.
- Carry out finite element simulations of polycrystalline molybdenum using artificial grain size distributions that are realizations of an assumed pdf of grain sizes.

### 5.3 Research Summary

A physics-based finite strain crystal plasticity constitutive model for BCC single crystals is developed to capture the strong temperature, rate, and orientation dependence of yield stress as well as the twinning–antitwinning asymmetry of the shearing resistance in these materials.

It is generally accepted that the mobility of screw dislocations controls the plastic flow in BCC metals. The motion of screw dislocations occurs primarily through the nucleation and the propagation of double-kinks along their lines; this is a thermally activated process (Tang et al., 1998. Acta Mater., 46, 3221–3235). Therefore, the theory of thermally activated motion of screw dislocations via nucleation of double kinks is adopted in the model to formulate the flow rule.

The response of the screw dislocation core to the externally applied stress is very complex. The critical stress to move a screw dislocation is affected not only by the usual resolved shear stress on the dislocation, but also by other stress components. Consequences of the latter are referred to as non-Schmid effects and lead to a strong orientation dependence of critical resolved shear stress and tension-compression asymmetry (Ito and Vitek, 2001. Phil Mag., 81, 1387–1407). A yield criterion that incorporates atomistically informed non-Schmid effects is used in the model.

The material constants in the model are determined by calibrating the model against existing experimental data on molybdenum. A systematic 2-step procedure is adopted for determination of these material constants without compromising their physical interpretation. The model is able to effectively describe the response of molybdenum crystals for different orientations and up to a homologous temperature of the order of 0.3 (Figs. 5.1 and 5.2).
The previously mentioned BCC crystal plasticity model is then extended by including the higher-order strain gradient terms, as discussed in Kuroda and Tvergaard (2008, J Mech Phys Solids, 56, 2573–2584). The implemented strain gradient crystal plasticity formulation involves higher-order governing equations and additional boundary conditions beyond the classical crystal plasticity theories. The additional boundary conditions enable the simulation of the hard boundaries that obstruct the plastic slip. This capability can be used to treat grain boundaries that are impenetrable to dislocations and hence allows simulating grain size effects explicitly.
Two material length-scale parameters are introduced in the model to capture the size effects in BCC metals. The first length scale is associated with hardening due to lattice curvature and nonuniform distribution of dislocations (such as dislocation pile-up at an obstacle) and is related to the second gradient of plastic strain. The second length scale is introduced in the model through dependence of slip resistance on the gradient of plastic slip through Taylor hardening, an approach similar to mechanism-based gradient theory of Han et al. (2005, J Mech Phys Solids, 53, 1188–1203).

The representative volume element is artificially constructed by centroidal Voronoi tessellation. This artificial template microstructure contains a sufficiently large number of grains such that essential information on microstructural and textural features can be represented. The finite element mesh with double nodes along the grain boundary was generated by OOF2 (2.0.5a6). The multiple finite-elements-per-grain approach is adopted.

Some preliminary finite element computations of polycrystalline molybdenum using representative volume element have been carried out. The effects of thermal softening and different ratios of length scale parameter to grain diameter on stresses and strains distribution are studied. The preliminary results suggest that a model can capture the size effects and thermal softening observed in BCC metals.

5.4 Collaborative Interactions

We have had very useful discussions with Rich Becker, Eric Klier, Brady Butler, and Bill deRosset on BCC behavior and modeling. We are collaborating with Mukul Kumar and Jeff Florando of the Lawrence Livermore National Laboratory on tantalum behavior and on collecting single crystal and polycrystal data on relatively pure BCC metals.

5.5 Publications and Presentations


3. Patil S. Modeling of BCC polycrystals; 2011 Jun 24; Presentation at Aberdeen Proving Ground, MD; Army Research Laboratory (US).
6. High-Rate Loading of Piezoelectric Ceramics

Core Faculty: KT Ramesh

ARL Collaborators: George Gazonas, Jim McCauley, David Lamb

Postdoctoral Fellow: Dr Leslie Lamberson

6.1 Long-Range Objectives

The overarching goal of this project is to analyze the interaction between loading dynamics and the electromechanical behavior of piezoelectric ceramics as a means of establishing relevant time and length scales associated with response. Model ceramics such as quartz, silicon carbide (SiC), and aluminum nitride (AlN) are considered in both modeling and experimental efforts in order to gain a fundamental understanding of coupled-field problems under dynamic loading regimes.

6.2 Objectives for July 1, 2010, to June 30, 2011

Third Quarter 2010:

- Perform additional Kolsky experiments on polycrystalline AlN and initial tests on single-crystal SiC to systematically and simultaneously measure electrical and deformation fields.

Fourth Quarter 2010:

- Compare results of piezoelectric ceramics tested under dynamic loading conditions (from crack initiation to complete material failure) with existing analytical model developed at the US Army Research Laboratory (ARL) (Wang et al., 2009. On the effective electroelastic properties of microcracked generally anisotropic solids. Int J Fract., 158:27–40).
  - Further develop model to estimate electromechanical performance specifically for ceramics of interest to this study as a function of damage, possibly considering inertial effects.
  - Measure quasi-static piezoelectric coefficients, both linear and, if possible, nonlinear, in model ceramics considered in experiments and modeling efforts (Penn State University facility).

First Quarter 2011:
- Perform normal plate impact experiments on cultured quartz samples to probe higher strain rate, coupled with electrical response behavior.

Second Quarter 2011:
- Perform normal plate impact experiments on polycrystalline AlN and single-crystal SiC (possibly single-crystal AlN) to probe higher strain rate, coupled with electrical response behavior.

6.3 Research Summary

6.3.1 Experimental Technique

Early efforts included developing a replicable and well-understood experimental technique to simultaneously measure the effective stress state and electrical response of a ceramic during dynamic loading. This technique involved vapor depositing 200 nm of pure aluminum in the loading direction faces of the ceramic test sample and matching paten faces to mitigate triboelectric noise or false polarization due to contact between the sample and (conductive) terminal device (Fig. 6.1).

![Fig. 6.1 Experimental technique for measuring dynamic electromechanical response of piezoelectric ceramics](image)

6.3.2 α - Quartz

Dynamic compression experiments at a strain rate of $10^3$ were performed on single-crystal x-cut α-quartz. While it had already been established that this material does not exhibit rate sensitivity (Kimberley et al., 2010. Visualization of the failure of quartz under quasi-static and dynamic compression, J Geophys Res., 115:B08207), to our knowledge no in situ results of the coupled electromechanical behavior using this experimental configuration has been previously reported in literature. Initial results showed that the electrical response initiates concurrently upon loading and follows conventional linear piezoelectric
theory yet appears to decline at a slower rate than the mechanical impulse during unloading (Fig. 6.2). This response manifests itself in generating piezoelectric stress coefficient “loops” when the charge is plotted as a function of the applied force (Fig. 6.3). No appreciable nonlinearities appeared in the electromechanical response for the type of loading and strain rate examined.

Fig. 6.2 Characteristic results of dynamic compression tests with plotted electromechanical response (left) and high-speed photography (right) performed on 5-mm cube of x-cut α-quartz

![Graph showing stress vs time and charge vs time](image)

Fig. 6.3 Characteristic piezoelectric “loop” illustrating effective charge as a function of the applied force during loading and unloading of the quartz sample. The slope of the line corresponds to the effective piezoelectric stress coefficient, d_{11}.
These experimental results were then compared to an established model developed at ARL for effective electroelastic properties of microcracked anisotropic solids and appear to follow the same trend—namely, that as the volume of damage increases in the material, so does the piezoelectric coefficient. However, further development and collaboration in modeling and experimental efforts between The Johns Hopkins University and ARL is necessary to fully understand the coupled-field interactions of quartz under the dynamic loading conditions examined.

6.3.3 Polycrystalline Aluminum Nitride

The same experimental technique was applied to samples of polycrystalline aluminum nitride. While the experimental conditions were identical, the results were highly inconsistent. Consequently, more conclusive testing is necessary to determine the electromechanical response of polycrystalline aluminum nitride or, rather, if a systematic or stochastic response is expected in such a ceramic. Qualitatively speaking, all test cases exhibited an initial electrical response that lagged the applied loading and did not fully decrease during unloading, as was seen in quartz. Most importantly, all cases showed a definitive piezoelectric response from the ceramic.

6.4 Collaborative Interactions

This work may take advantage of interactions with Penn State University’s work on piezo electromagnetic coupling in ceramics.

6.5 Publications and Presentations

7. **Administration, Education, Training, and Collaborative Structures**

Hopkins Coordinator: KT Ramesh

ARL Coordinators: J McCauley, RJ Dowding

### 7.1 Long-Range Objectives

The long-range objective is to develop a collaborative research structure with significant educational benefits to both US Army Research Laboratory (ARL) and Johns Hopkins.

### 7.2 Objectives for July 2010 to June 2011

Third Quarter 2010:

- Bring together ARL staff and Hopkins faculty and students in Center Seminars.

Fourth Quarter 2010:

- Bring together ARL staff and Hopkins students and faculty in Collaborative Research Group meetings.

First Quarter 2011:

- Bring together ARL staff and Hopkins faculty and students in a Center Seminar.

Second Quarter 2011:

- Bring together ARL staff and Hopkins students and faculty in Collaborative Research Group meetings.

### 7.3 Accomplishments

The various groups are meeting regularly, and the seminar series is running well. Invited CAMCS seminar speakers in this period are listed in the following Table.
<table>
<thead>
<tr>
<th>SPEAKER</th>
<th>ABSTRACT</th>
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<tr>
<td>Shailendra P. Joshi</td>
<td>Nonlocal Continuum Crystal Plasticity with Internal Residual Stresses</td>
<td>June 25, 2010</td>
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<tr>
<td>Douglas J. Bammann</td>
<td>Towards a Consistent Thermodynamic Theory of Multiscale Inelastic Deformation</td>
<td>December 10, 2010</td>
</tr>
<tr>
<td>Dimitris C. Lagoudas</td>
<td>Recent Advances in SMA-Based Aerospace Structures</td>
<td>May 10, 2011</td>
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<tr>
<td>Dhirendra V. Kubair</td>
<td>Computational Dynamic Fracture of Inhomogeneous Materials</td>
<td>May 18, 2011</td>
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8. List of Theses, Publications, and Presentations

8.1 Publications


8.2 Presentations


5. Li B, et al., Extended zonal dislocations mediating twinning in titanium. TMS. 2011; San Diego, CA.

6. Li B, et al., Twinning without a twinning plane. TMS. 2011; San Diego, CA.

7. Daphalapurkar NP, Ramesh KT. Partial dislocations and deformation twinning in pure face-centered cubic metals. Conference presentation. MS&T. 2010 Oct; Houston, TX.

8. Daphalapurkar NP, Ramesh KT. Partial dislocation nucleation and twinning in aluminum. TMS Annual Meeting and Exhibition. 2011 Mar; San Diego, CA.


15. Patil S. Modeling of BCC polycrystals; 2011 Jun 24; Presentation at Army Research Laboratory (US), Aberdeen Proving Ground, MD.