Mesoscale Modeling of Microstructure Evolution During Large Plastic Deformations

Gorti B. Sarma and B. Radhakrishnan

Oak Ridge National Laboratory
Oak Ridge, TN 37831-6359

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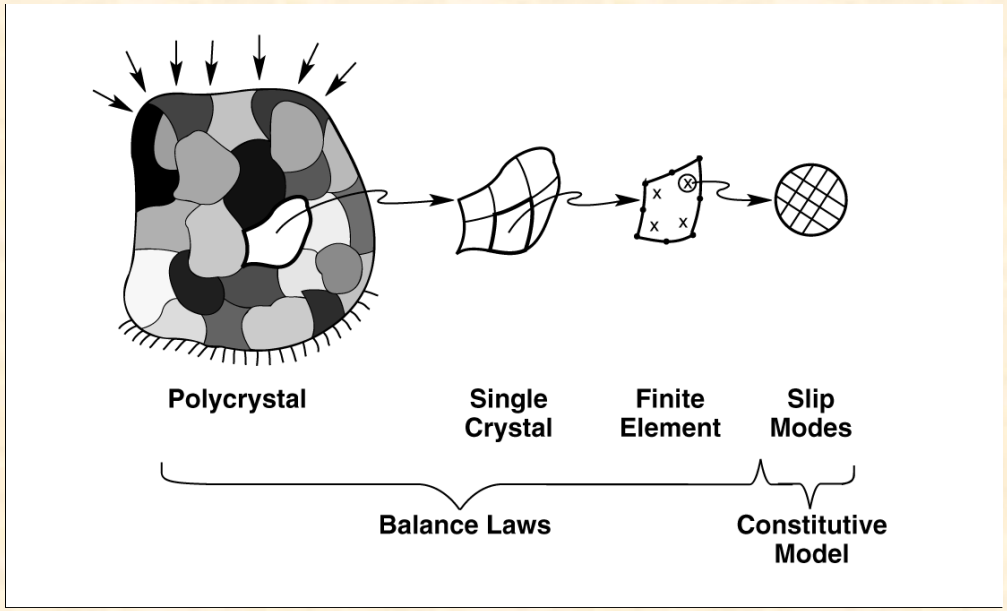
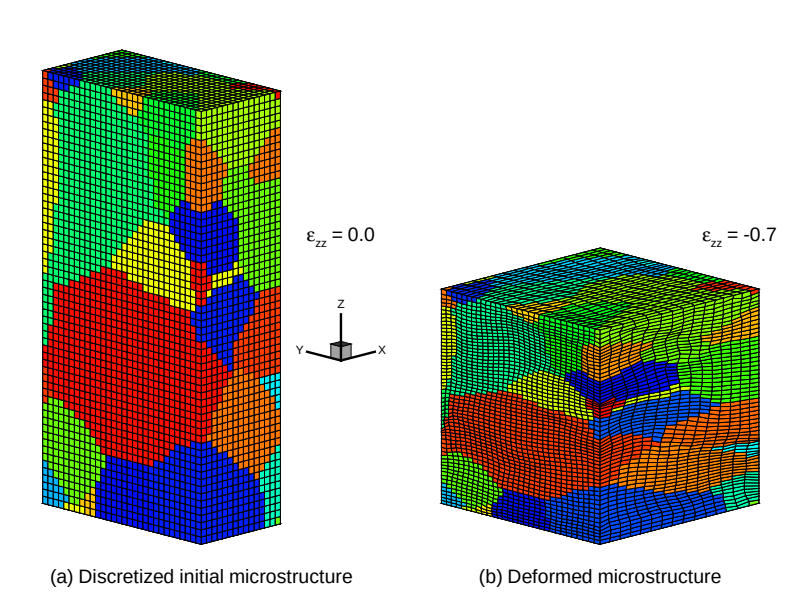
Finite Element Method is used in Conjunction with Crystal Plasticity to Model Deformation at the Mesoscale





- Discretization carried out directly at the grain level to model non-uniform deformations due to grain interactions
- Material constitutive behavior modeled using crystal plasticity to capture anisotropic response and texture evolution
- Formulation implemented on parallel computers to enable simulations using large, three-dimensional meshes

Crystal Plasticity Provides the Framework for Modeling Plastic Deformation by Slip

- Power law relates slip system shearing to resolved shear stress
- Schmid orientation tensor is used to relate
  - Crystal deformation rate to slip system shearing rates
  - Crystal stress to slip system resolved shear stress
- Non-linear constitutive relation between stress and deformation rate is solved to obtain the slip system shear rates

$$\tau^{\alpha} = \tau_{cr} \frac{\dot{\gamma}^{\alpha}}{\dot{\gamma}_0} \left| \frac{\dot{\gamma}^{\alpha}}{\dot{\gamma}_0} \right|^{m-1}$$

$$\mathbf{D}_{\mathrm{c}} = \sum_{\alpha} \mathbf{P}^{\alpha} \dot{\gamma}^{\alpha}$$

$$\tau^{\alpha} = \sigma_{ij} n_j^{\alpha} s_i^{\alpha} = \sigma \cdot (\boldsymbol{s}^{\alpha} \otimes \boldsymbol{n}^{\alpha})$$

$$\mathbf{D}_{\mathrm{c}} = \left[\sum_{\alpha} \left| \frac{\boldsymbol{\sigma} \cdot \mathbf{P}^{\alpha}}{\tau_{cr}} \right|^{\frac{1}{m}-1} \frac{\dot{\gamma}_0}{\tau_{cr}} \mathbf{P}^{\alpha} \otimes \mathbf{P}^{\alpha} \right] \boldsymbol{\sigma}$$

Evolution Laws for Crystal Orientation and Slip System Strength Model Texture Evolution and Strain Hardening

- Reorientation of crystal lattice is computed from difference between crystal spin and plastic spin due to slip system shearing

$$\dot{\mathbf{R}}^* = \left(\mathbf{W}_c - \sum_\alpha \mathbf{Q}^\alpha \dot{\gamma}^\alpha \right) \mathbf{R}^*$$

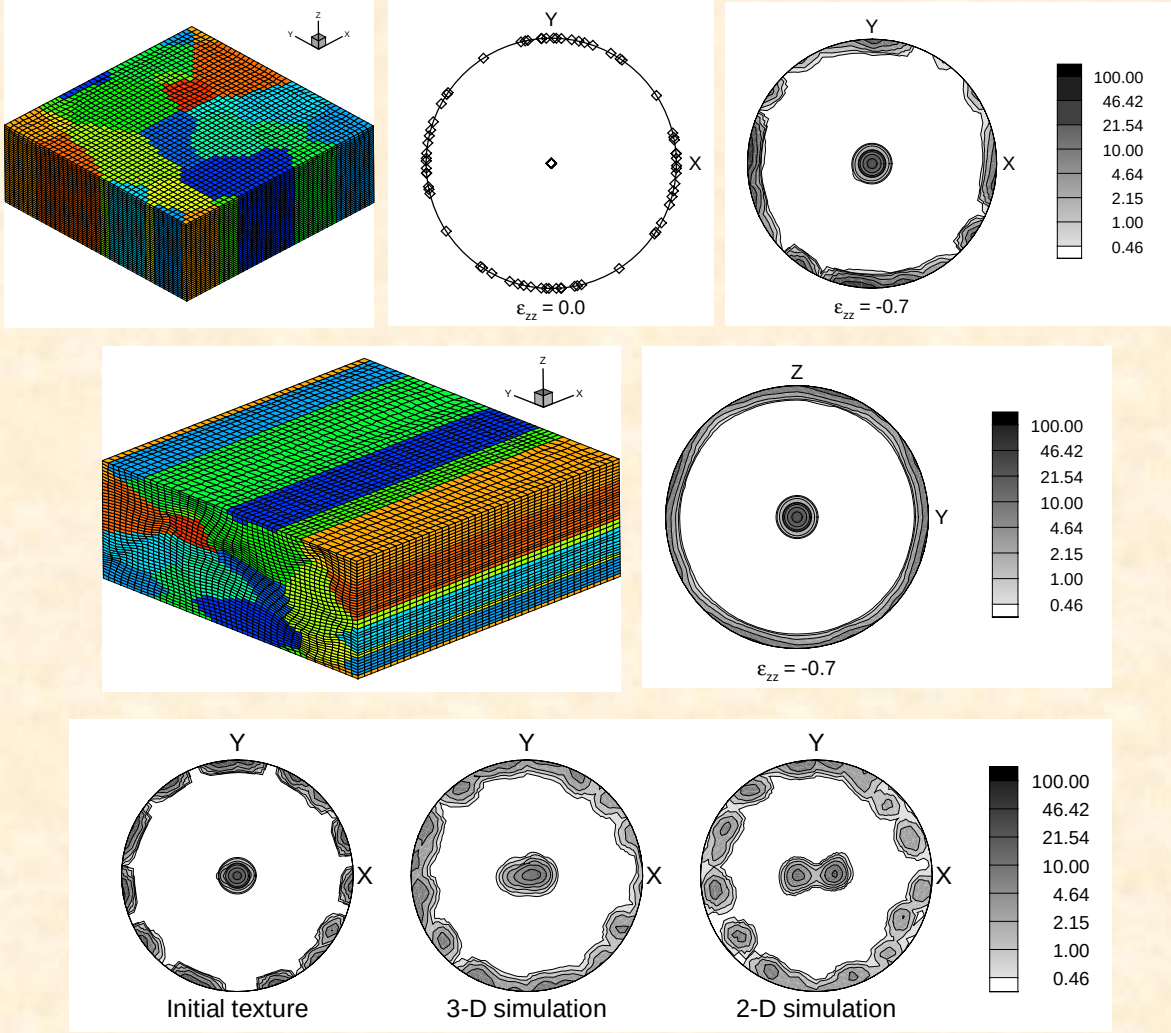
- Strain hardening is modeled through evolution of slip system strength

$$\dot{\tau}_{cr} = H_0 \left(\frac{\tau_{cr}^s - \tau_{cr}}{\tau_{cr}^s - \tau_{cr}^0} \right) \sum_\beta \left| \dot{\gamma}^\beta \right|$$

- Increase in stored energy at each step is proportional to incremental work done at the slip system level

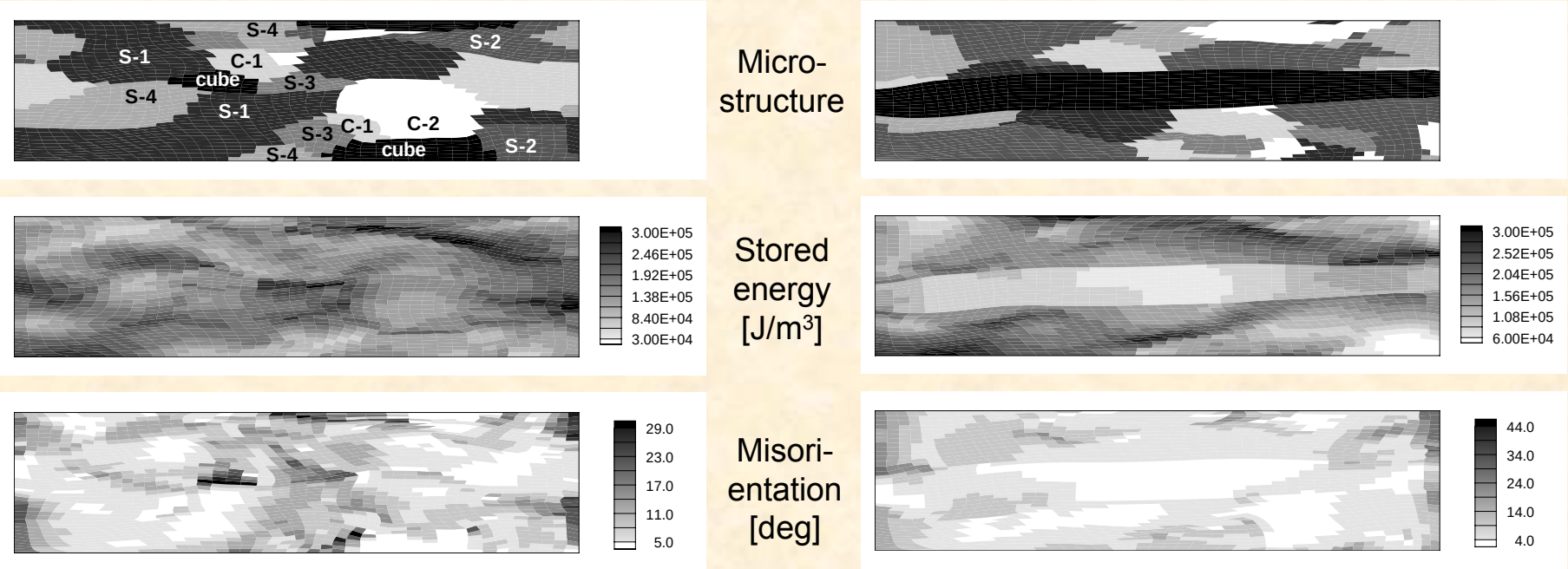
$$\Delta \tau_{cr} \sum_\beta \left| \dot{\gamma}^\beta \right| \Delta t$$

Mesoscale Modeling of Columnar Microstructures Shows Heterogeneity of Deformation and Texture Evolution



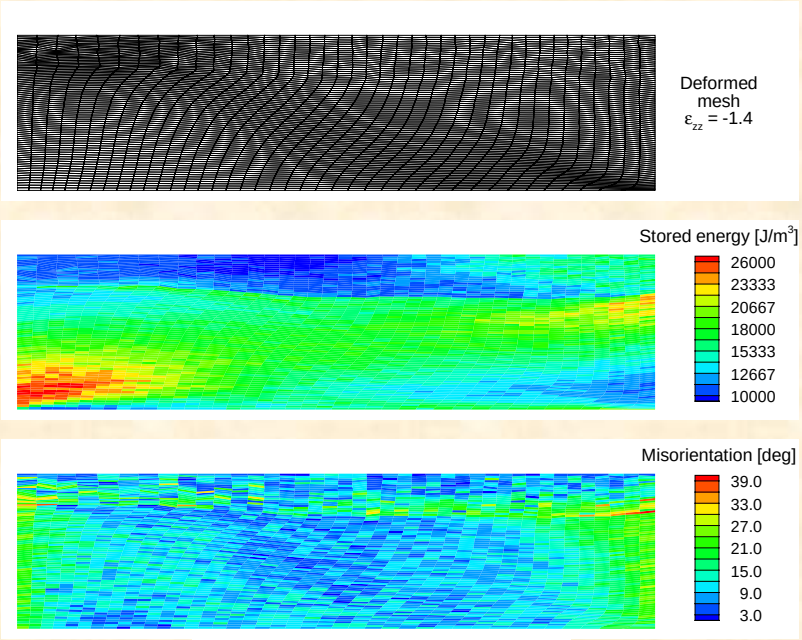
- Columnar grains aligned with compression axis deform with minimal rotation
- Columnar grains normal to compression axis show considerable rotation about easy growth direction
- 2D and 3D simulations show significant differences in texture evolution

Mesoscale Model Has Been Applied to Hot Deformation of Microstructures Containing Cube-oriented Grains

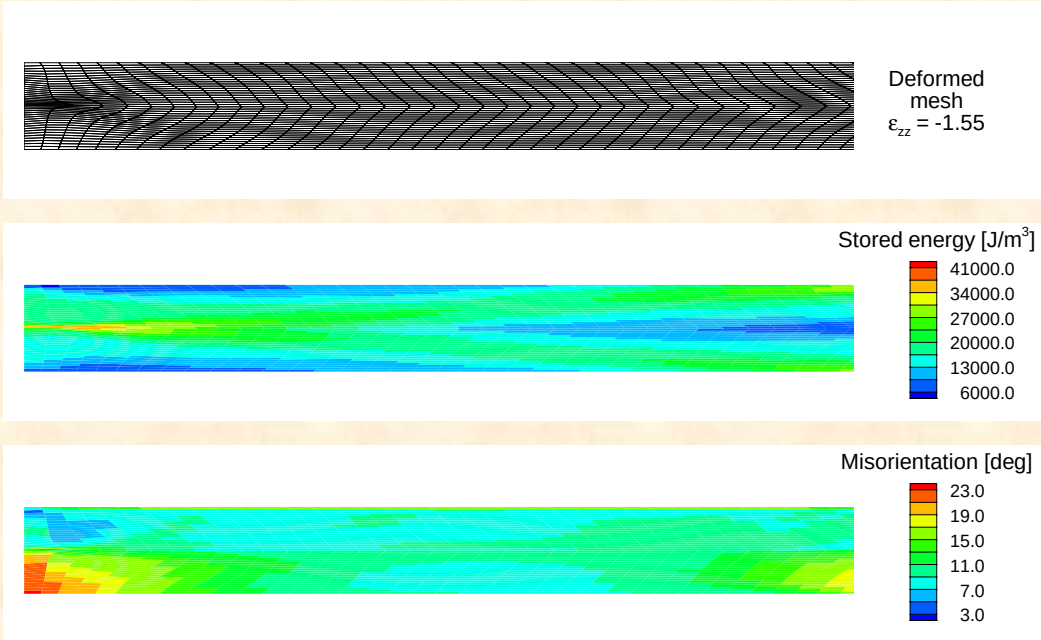


- Microstructures deformed in plane strain compression to 50% reduction
- Stored energy on cube grain side is lower along flat elongated boundaries parallel to the extension direction
- Misorientation from initial cube was low near boundaries parallel to, and high along boundaries perpendicular to, the extension direction

Plane Strain Compression of Aluminum Bicrystals Under Hot Deformation Conditions Has Been Modeled



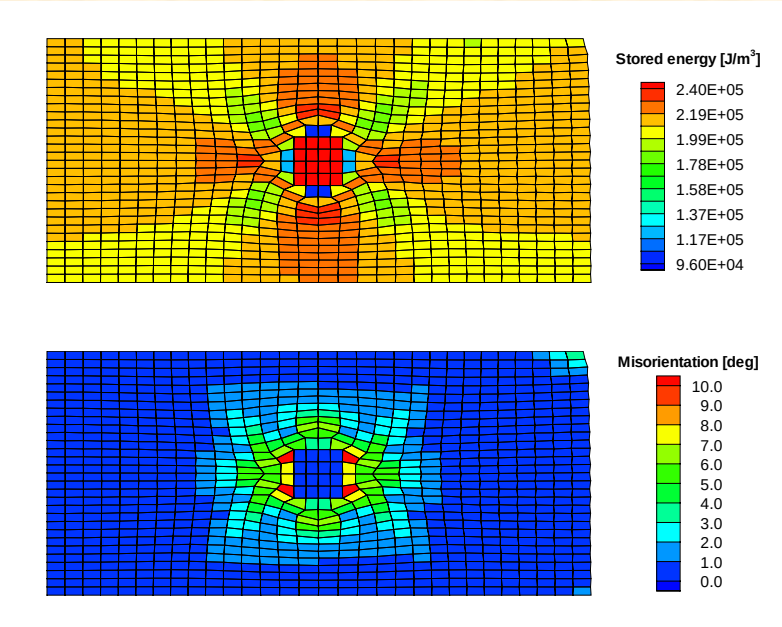
cube-S bicrystal

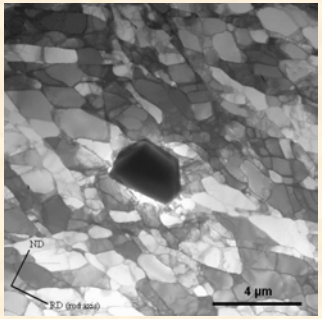


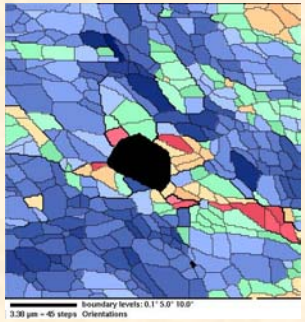
copper-S bicrystal

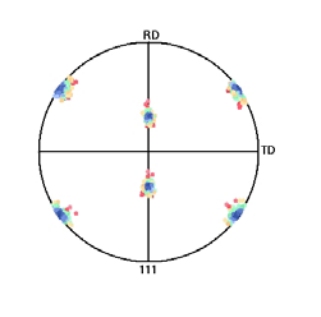
- Different combinations of crystals with orientations of ideal rolling texture components were simulated: cube-S, copper-S and brass-S
- Simulations of cube-S bicrystal showed lower stored energy in cube, and fairly small misorientation from initial orientation for both cube and S
- Simulations of copper-S bicrystal showed similar stored energy misorientation distributions for both copper and S

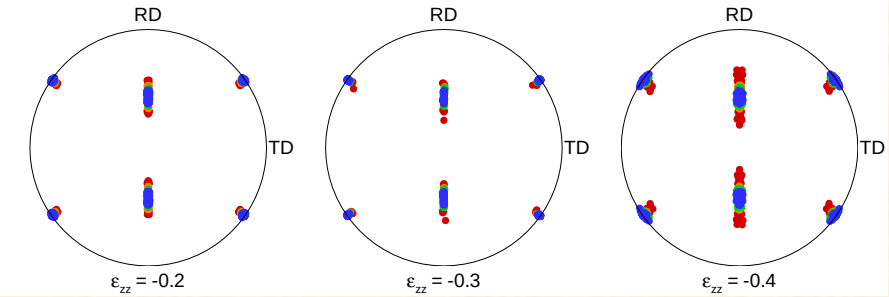
Modeling of Goss-oriented Single Crystal of Al Containing a Hard Particle Captures Formation of Deformation Zone











- Stored energy and misorientation from initial Goss orientation are higher in a region of enhanced deformation around the second phase particle
- Reorientation of the initial Goss orientation by rotation about the transverse direction during plane strain compression is captured by the model, matching the spread seen in experiments

Conclusions and Summary

- Finite element method has been used to simulate the heterogeneous deformation of metallic materials at the mesoscale through explicit discretization of the individual grains
- Use of crystal plasticity enables the model to capture the evolution of grain orientation and slip system strength
- Mesoscale modeling has been applied to various types of microstructures
  - Bicrystals and polycrystals
  - Single crystals with hard particles
  - Microstructures with columnar grains
- Mesoscale deformation model can be easily extended to
  - Other crystal structures (eg. bcc, hcp)
  - Polyphase materials

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