Effect of Finite Element Discretization on Texture Predictions Using Mesoscale Simulations of Deformation and Recrystallization

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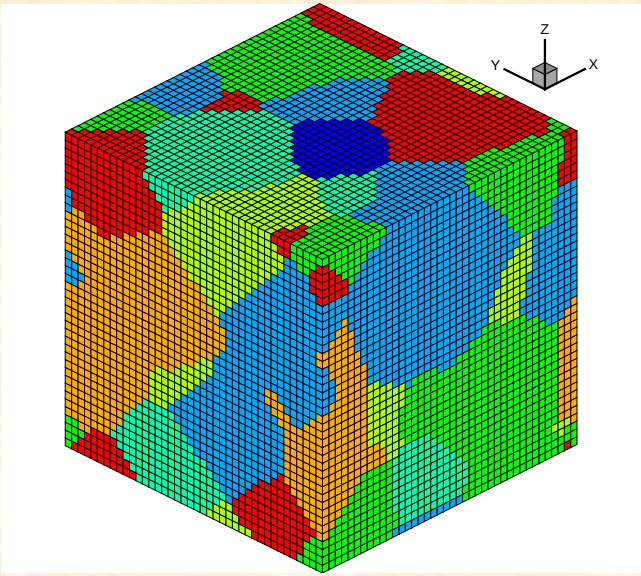
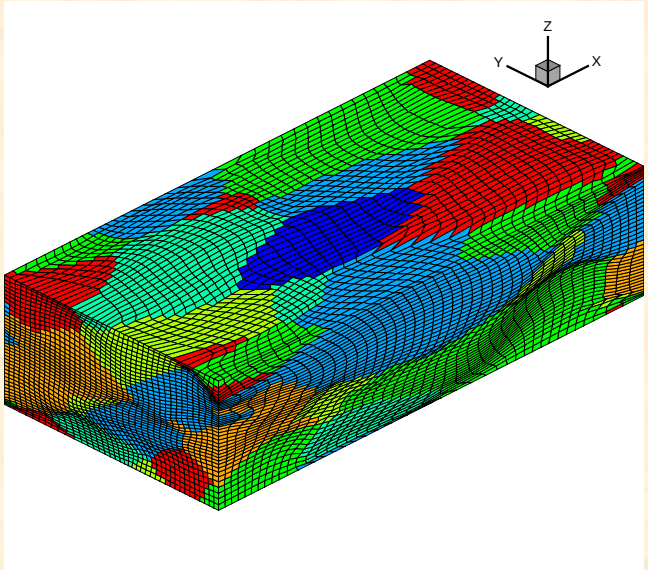
Background and Objective

- Aluminum alloys containing micron-size particles form localized deformation zones
  - Region of higher stored energy and misorientations
  - Source of particle stimulated nucleation (PSN)
- Nuclei that form in deformation zone can significantly alter the recrystallization texture and kinetics
- Objective of research is to use a coupled finite element-Monte Carlo technique to investigate the deformation and recrystallization of particle-containing aluminum alloys
  - Effect of the level of finite element discretization
  - Microstructure, texture and kinetics with and without particle
  - Effect of shape and microstructural location of particle

Finite Element Method Coupled With Crystal Plasticity Was Used to Model Deformations 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 a massively parallel computer 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

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

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

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

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

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

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

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

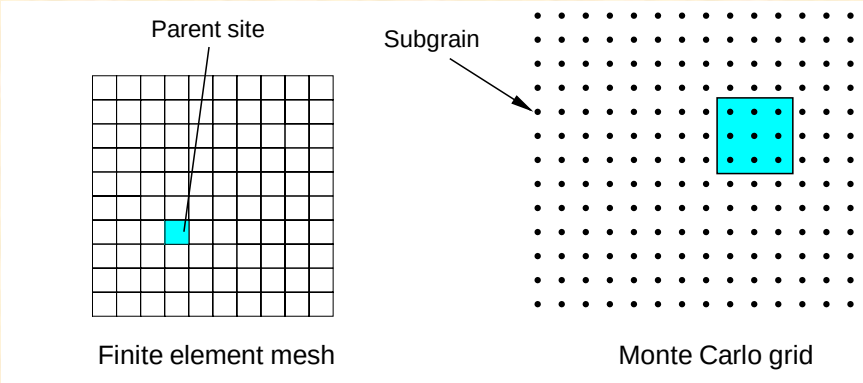
- Strain hardening is modeled through evolution of slip system strength

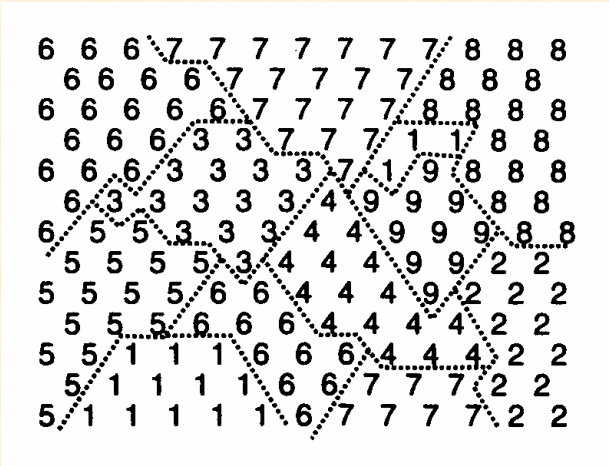
$$\dot{\tau}_{cr} = H_0 \left(\frac{\tau_{cr}^s - \tau_{cr}}{\tau_{cr}^s - \tau_{cr}^0} \right) \sum_\beta \left| \dot{\gamma}^\beta \right|$$

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

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

Finite Element Model is Coupled with Monte Carlo Technique for Evolving Microstructure and Texture



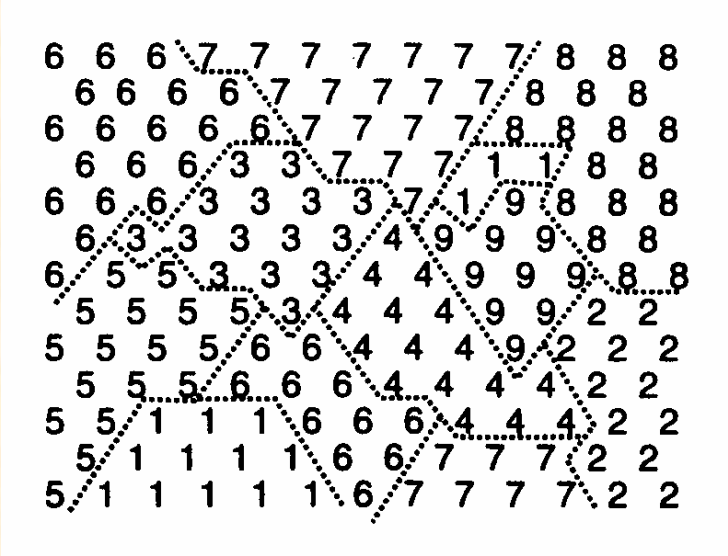


- Microstructural deformation is modeled using FE technique to capture non-uniform stored energy and orientation distributions
- Deformation substructure, assumed to be in the form of well developed subgrain structure, is extracted from FE results

$$H = \frac{\gamma}{2d}\left[\frac{\Delta\theta}{\theta^*}\left(1 - \ln\frac{\Delta\theta}{\theta^*}\right)\right]$$

- Deformation substructure is evolved using a Monte Carlo technique to model kinetics, microstructure and texture

Monte Carlo Simulation of Substructure Evolution – Recrystallization by Abnormal Subgrain Growth



$$E = \frac{1}{2}\sum_{i}^{n}\sum_{j}^{NN} J(S_i S_j)(1-\delta_{S_i S_j})$$

$$N_{MCS}^{\mu\gamma} = N_{MCS}\frac{\mu\gamma}{\mu_{max}\gamma_{max}}$$

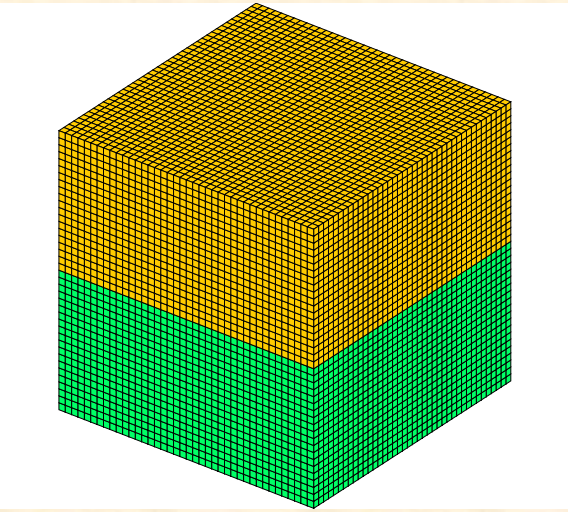
$$p(S_i, S_j, \Delta E, T) = \begin{bmatrix} 1 & \Delta E \le 0 \\ exp(-\Delta E / kT) & \Delta E > 0 \end{bmatrix}$$

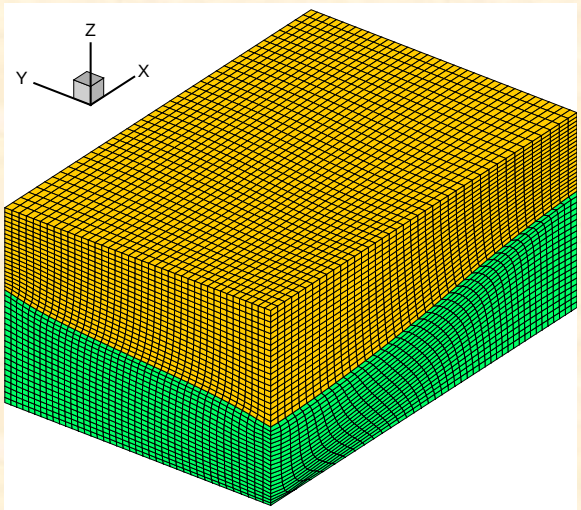
- No bulk stored energy term
- Discretized subgrain structure is represented by orientation numbers
- Each number stands for a crystallographic orientation in the form of an axis-angle pair
- Subgrain boundaries are assumed to exist across sites with unequal numbers
- Grain boundary character is described by misorientation between boundary sites

Coupled Mesoscale Model Was Applied to Single Crystals and Bi-crystals

- Discretizations consisted of a cube shaped domains with 40, 50, 60 or 80 elements along each side
- Single crystals of different orientations and with different shapes for hard particles were modeled
  - Cube (001)[100], S (123)[$\underline{6}$ $\underline{3}$ 4], and Copper (112)[$\underline{1}$ $\underline{1}$ 1]
  - Spherical, cube and rotated cube particles
- Bi-crystals with and without a spherical hard particle at the grain boundary were modeled
  - S-Cube, S-Copper, and Copper-Cube bi-crystals
- Hard particle was modeled by setting the slip system strength of associated elements above the saturation value

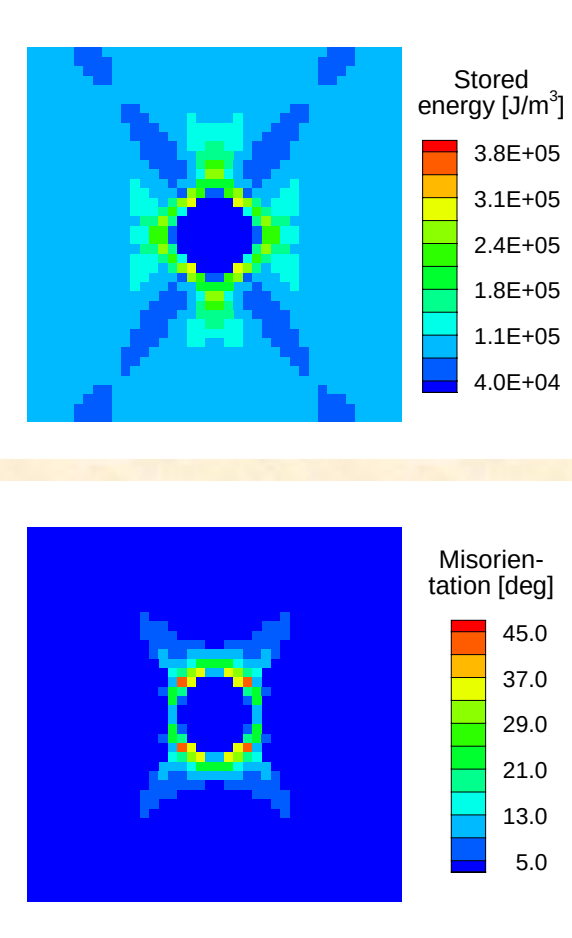
Plane Strain Compression of Microstructures Under Hot Deformation Conditions Were Simulated



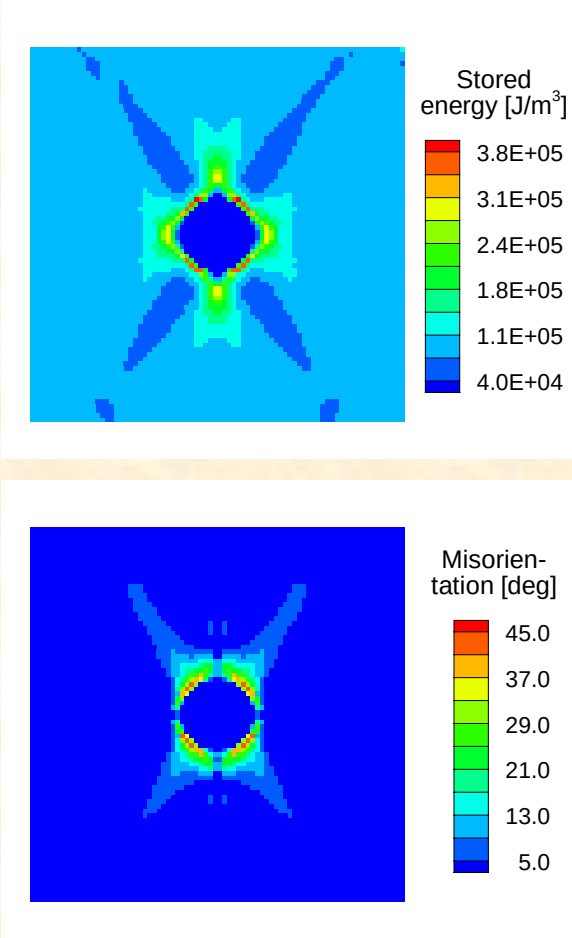


- Material was assumed to have FCC crystal structure
- Material parameters were obtained by fitting compression test data for aluminum deformed at 400°C at various strain rates
- Deformation under elevated temperature was modeled assuming slip on non-octahedral {110} planes in addition to {111} planes
- Microstructures were deformed to 40% reduction in height

Stored energy and misorientation distributions for Cube oriented grain with spherical hard particle



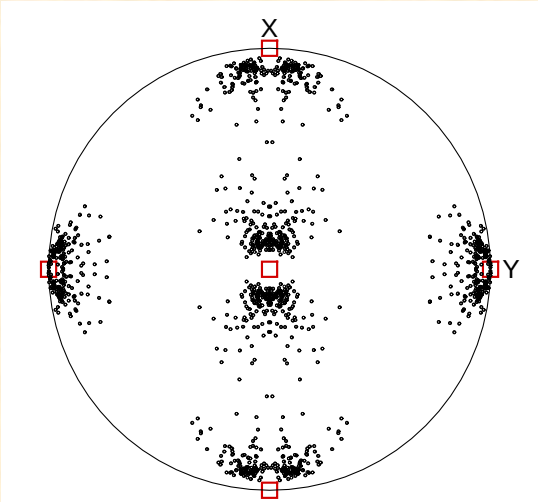
40 elements



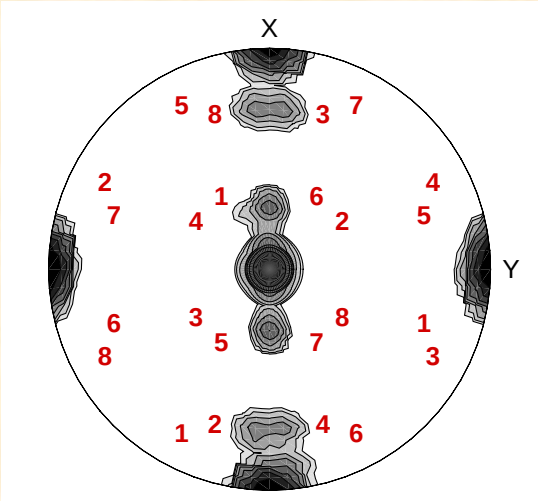
80 elements

- Simulations are able to capture formation of deformation zone around the particle
- Misorientations from initial Cube are high (~ 40°) close to particle
- Mesh refinement improves ability to capture variations in stored energy and misorientation

Cube oriented grain with hard particle shows some TD rotated components after recrystallization



After deformation

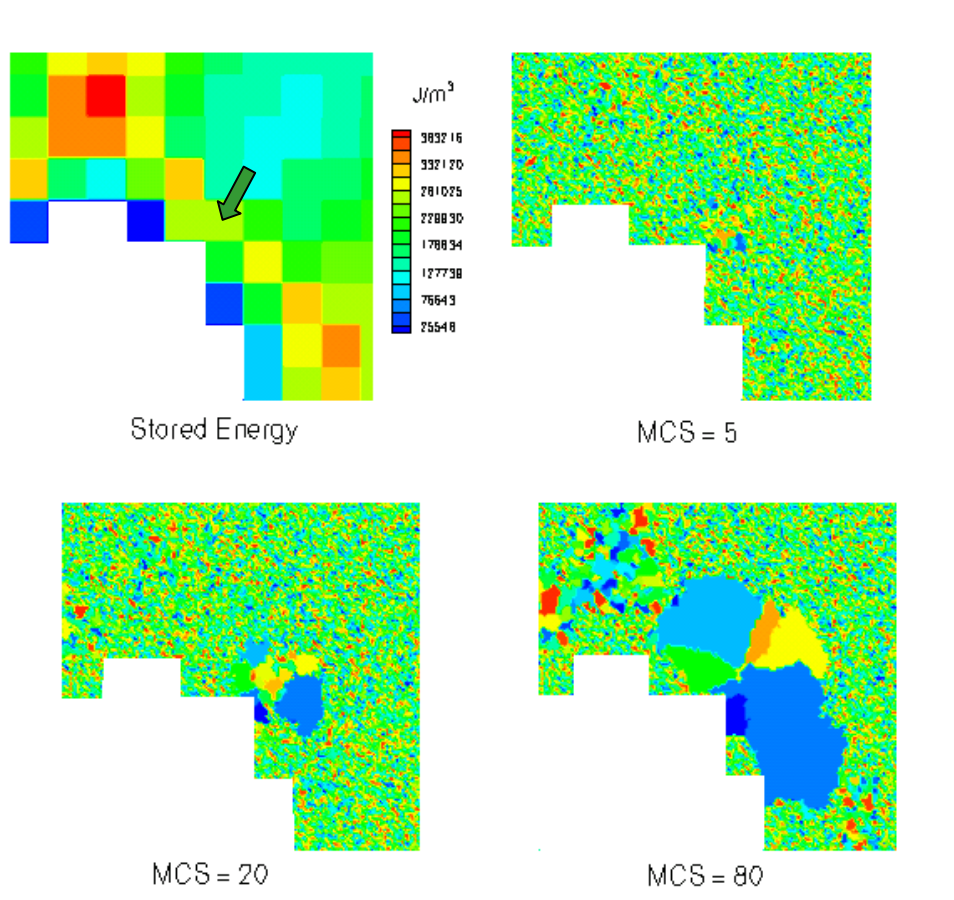


After recrystallization

Number	Rotation axis
1	111
2	111
3	111
4	111
5	111
6	111
7	111
8	111

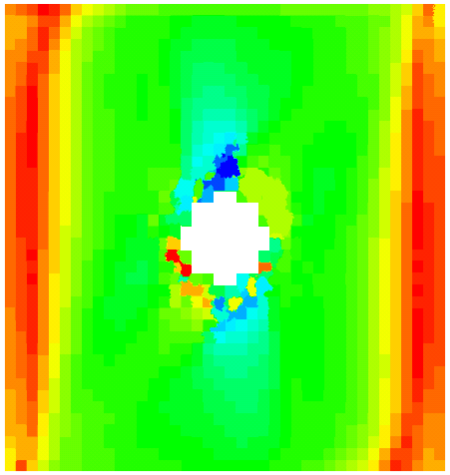
- Only elements that are misoriented by more than 5° from cube (deformation zone) are shown in deformation texture
- Recrystallized texture does not coincide with any of the 40°<111> rotations of Cube

Simulation of S oriented grain with hard particle captures micro-growth orientation selection of nuclei

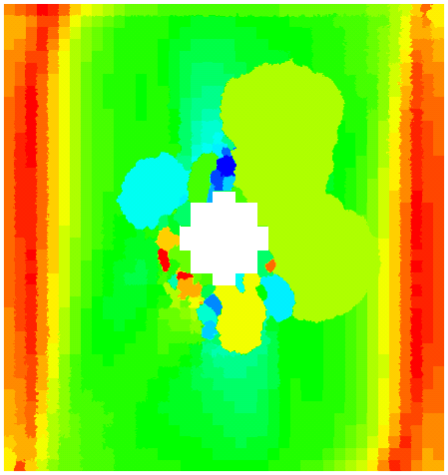


- Element marked by arrow has 40°<111> misorientation with respect to surrounding elements
- Initial stored energy within the element is greater than in most neighboring elements
- Recovery by abnormal subgrain growth is aided by special boundaries and occurs rapidly within the element
- When the energy within the element is lower than outside, the subgrains become potential nuclei

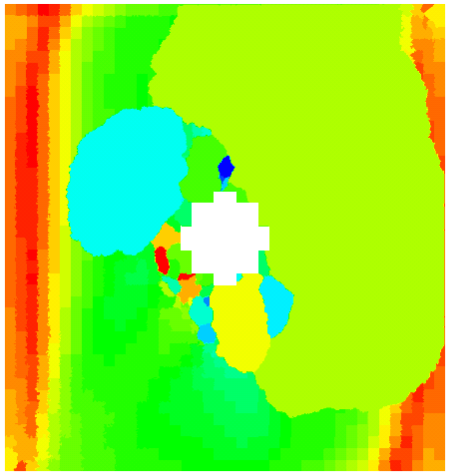
Temporal evolution of recrystallization for S oriented grain in the presence of spherical hard particle



MCS = 80



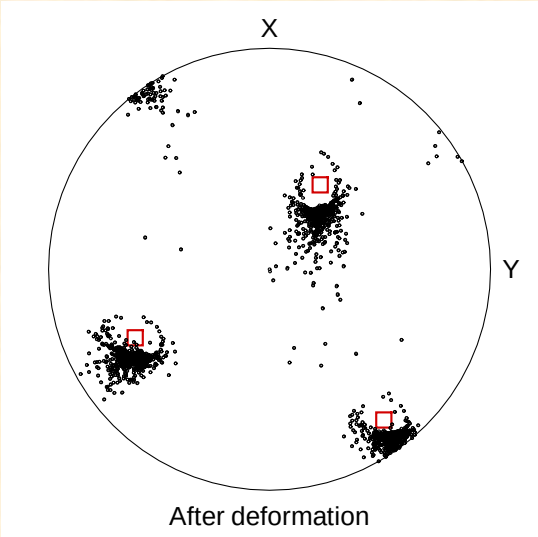
MCS = 400

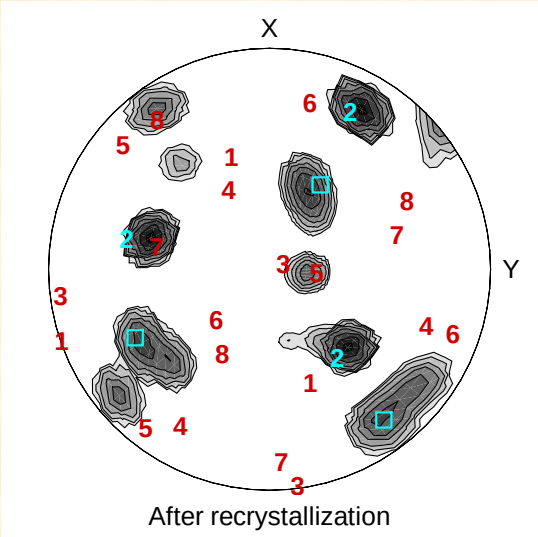


MCS = 800

- Rapid growth of particle stimulated nucleus formed by micro-growth selection with 40°<111> misorientation
- Many other potential “nuclei” form but their growth is overcome by the growth of the special nucleus
- Recrystallization texture is dominated by the orientation of the special nucleus

S oriented grain with spherical hard particle shows strong 40°<111> recrystallization texture

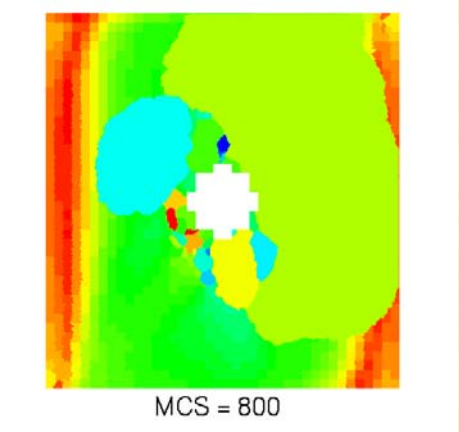




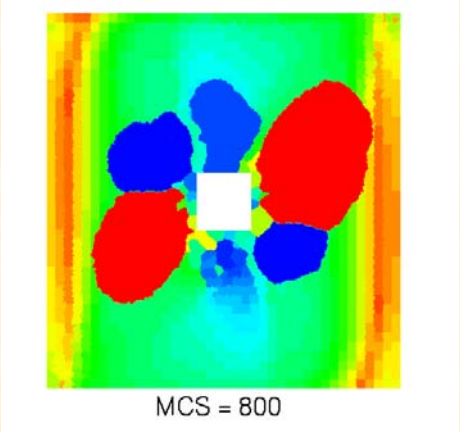
Number	Rotation axis
1	111
2	**$\underline{1}$11**
3	1$\underline{1}$1
4	11$\underline{1}$
5	1$\underline{11}$
6	$\underline{1}$1$\underline{1}$
7	$\underline{11}$1
8	$\underline{111}$

- Only elements deviated by more than 5° from S (deformation zone) are shown after deformation
- Significant increase in intensity of an orientation very close to 40°[$\underline{1}$11] rotation of S is observed
- Rex. texture also includes weaker "random" components not misoriented by 40°<111> from S

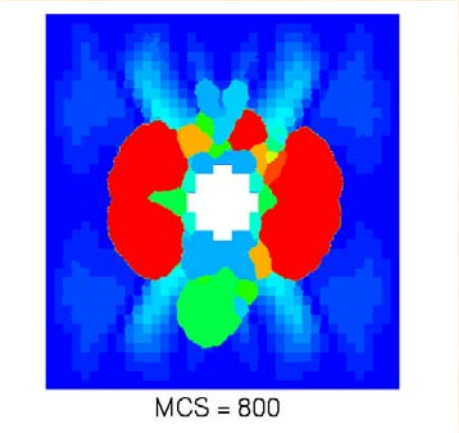
Initial crystal orientation and particle shape affect the number and spatial distribution of nuclei



S orientation with spherical particle



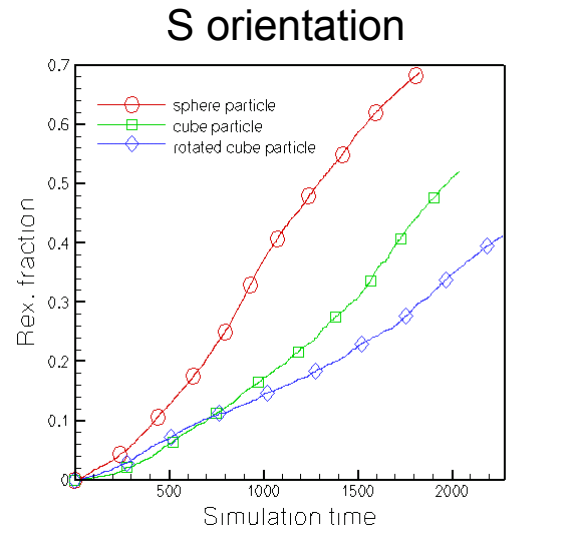
S orientation with cube shaped particle

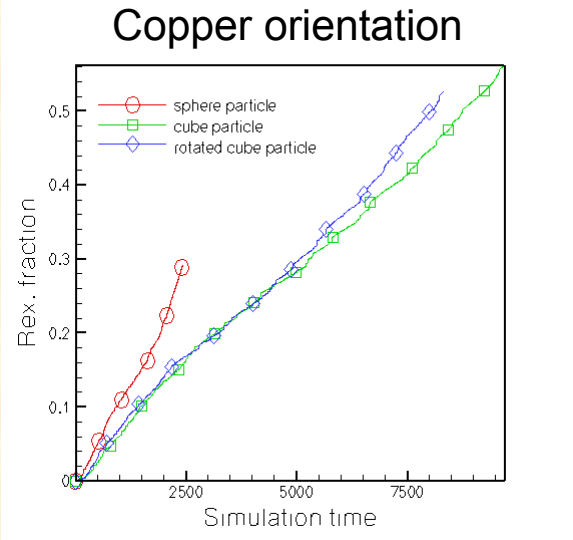


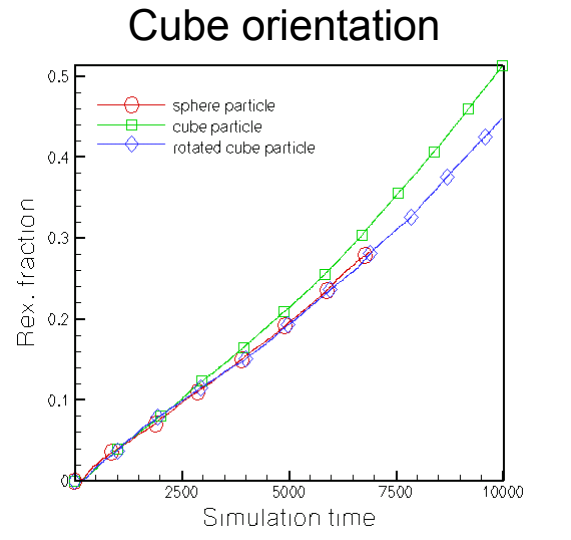
Cube orientation with spherical particle

- Initial orientation determines the number of active slip systems, and the orientation of slip systems with respect to the compression axis
- Particle shape determines the extent of slip-shadowing in regions very close to the particle

Effect of particle shape and initial orientation are seen in the recrystallization kinetics

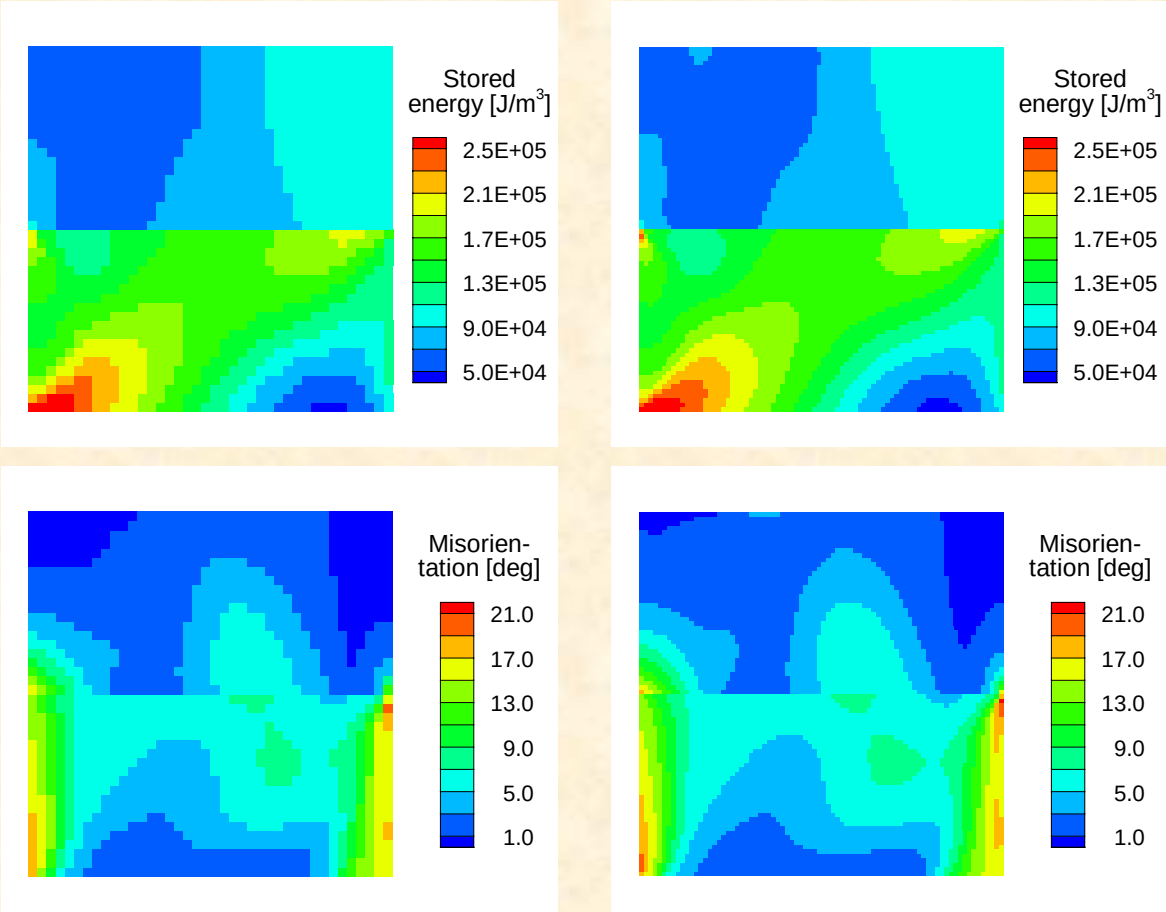






- All particle shapes produced nuclei with special 40°<111> misorientation for the S oriented crystal, leading to faster kinetics
- Only spherical particle produced specially oriented nuclei for the crystal initially at Copper orientation
- None of the particle shapes produced specially oriented nuclei for the crystal initially at Cube orientation

Stored energy and misorientation distributions for the S-cube bi-crystal

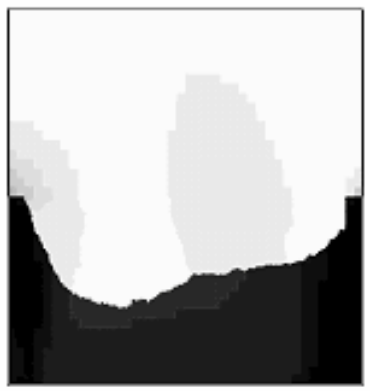


40 elements

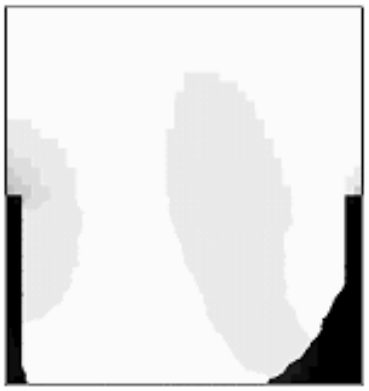
80 elements

- Stored energy is lower in the cube grain than in S, especially along the interface
- Misorientations from initial cube and S are fairly low, except near the edges for S
- Mesh refinement improves ability to capture variations in stored energy and misorientation

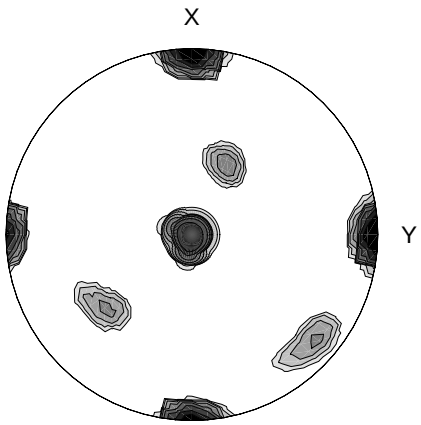
S-Cube bi-crystal shows strong Cube texture after recrystallization



MCS = 400



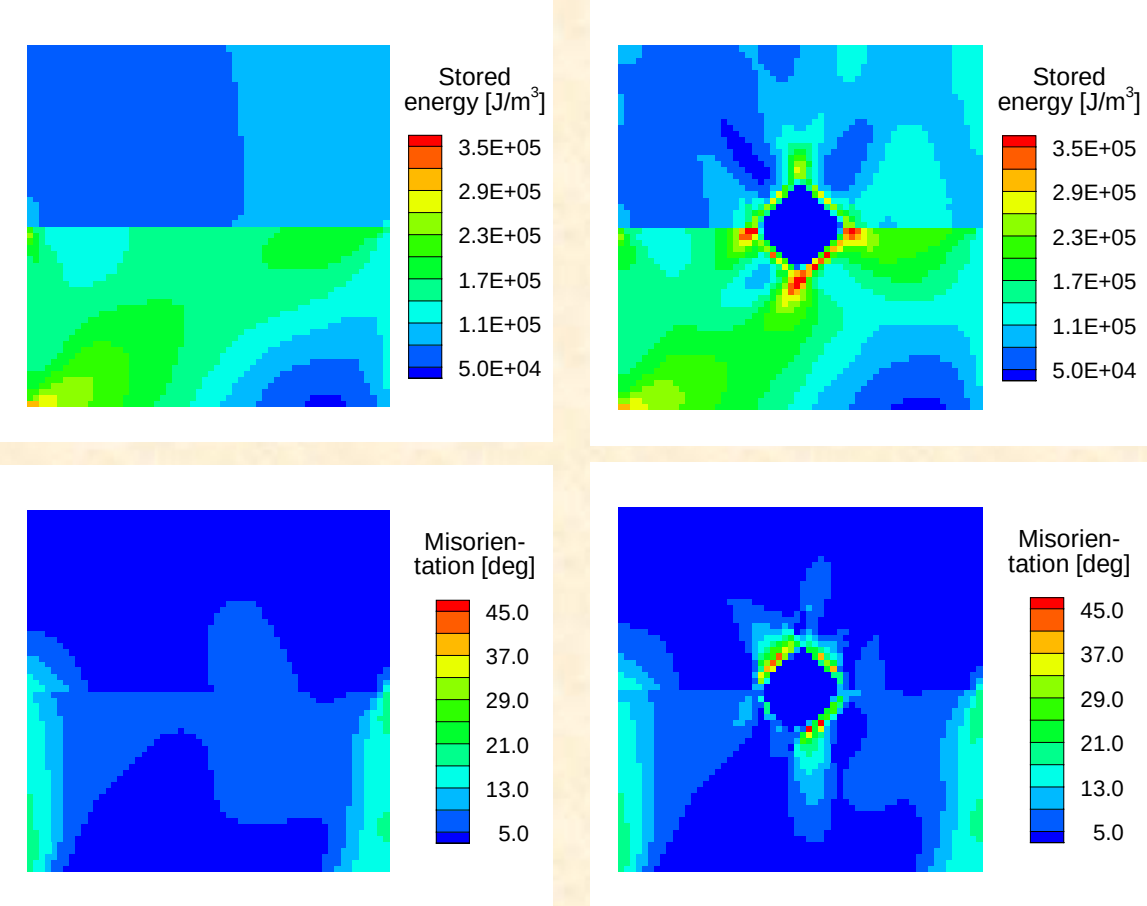
MCS = 1200



After recrystallization

- Lower stored energy on Cube side causes growth of Cube grain into S by strain induced boundary migration (SIBM)
- Growth of cube grain is aided by special 40°<111> misorientation between Cube and S

Stored energy and misorientation distributions for S-cube bi-crystal with spherical hard particle

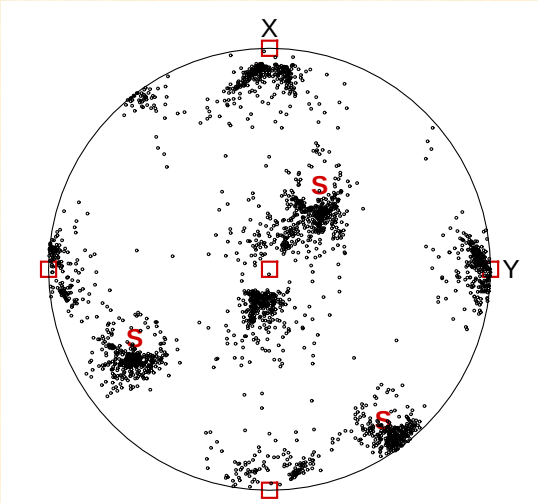


Without particle

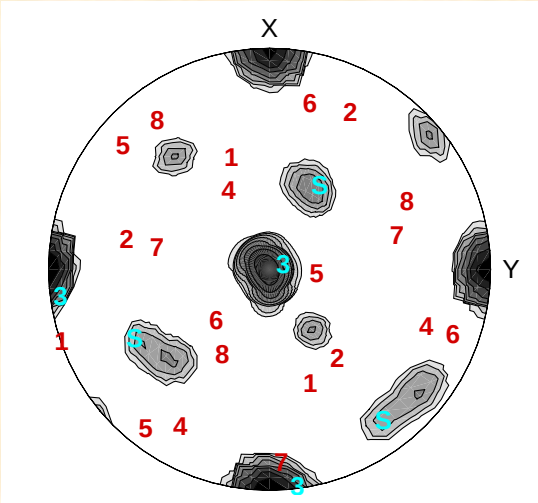
With particle

- Stored energy is lower in Cube grain compared to S
- Stored energy is higher in the deformation zone close to the particle
  - Stored energy is higher on S side near the particle
- Misorientation from the initial orientation is much higher in the vicinity of the particle

S-Cube bi-crystal with hard particle shows strong Cube texture after recrystallization



After deformation

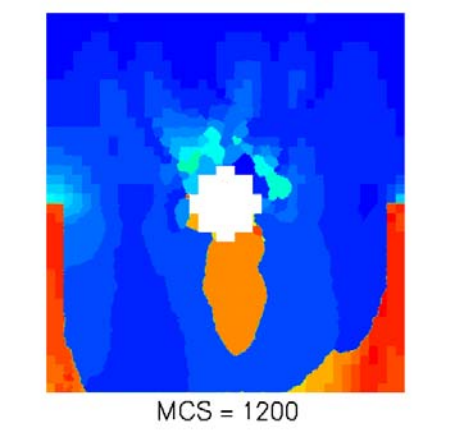


After recrystallization

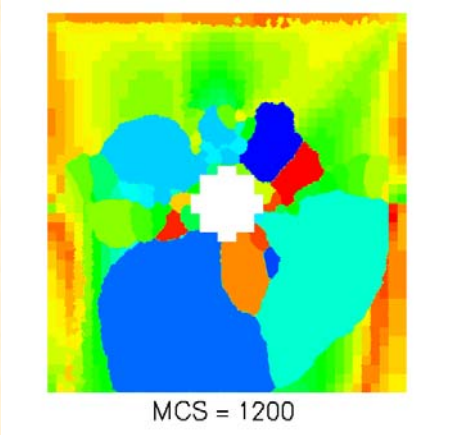
Number	Rotation axis
1	111
2	$\underline{1}$11
3	**1$\underline{1}$1**
4	11$\underline{1}$
5	1$\underline{11}$
6	$\underline{1}$1$\underline{1}$
7	$\underline{11}$1
8	$\underline{111}$

- Recrystallized texture has a strong 40°[1$\underline{1}$1] rotation of S
  - Corresponds to misorientation between Cube and S (migration of interface)
- Particle stimulated nucleation contributes weaker “random” components

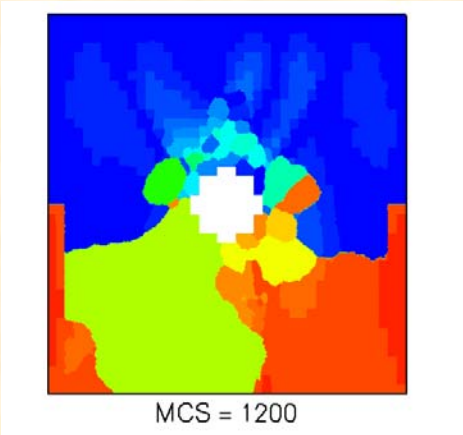
Hard particle at bi-crystal boundary can have significant effect depending on grain orientations



Cube-S



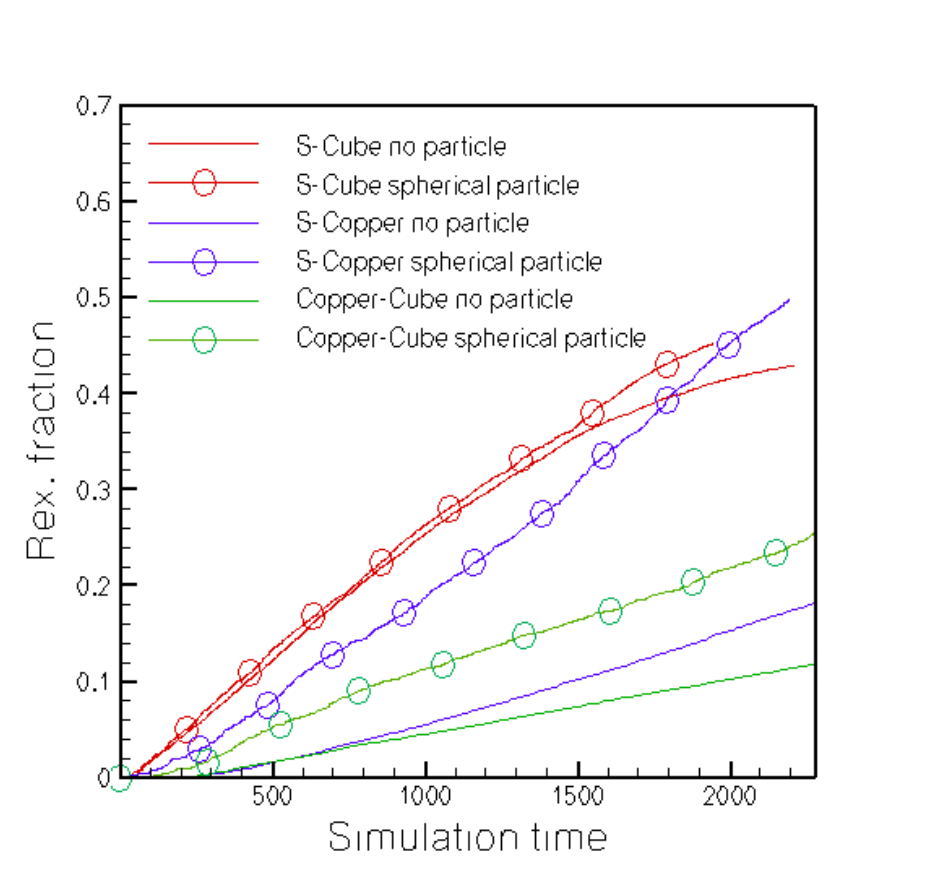
Copper-S



Cube-Copper

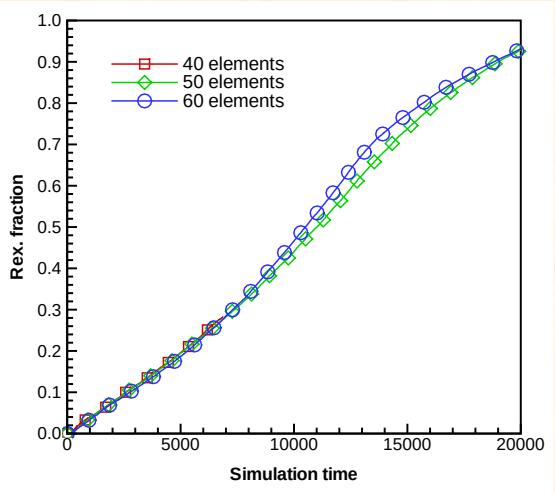
- No significant effect due to particle for S-Cube bi-crystal
  - Nucleus produced in the S grain is overtaken by migration of Cube-S interface
- Significant effect for S-Copper and Copper-Cube bi-crystals
  - Special nuclei form in S grain for Copper-S bi-crystal and in Copper grain for Cube-Copper bi-crystal

Recrystallization kinetics of bi-crystals is significantly enhanced in the presence of particles

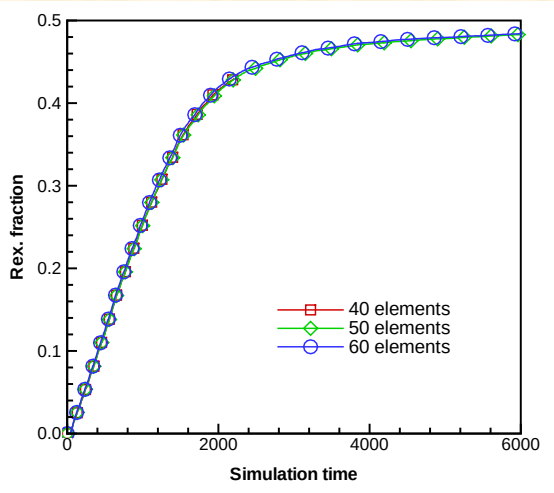


- Cube-Copper and S-Copper bi-crystals containing particles recrystallize faster than particle-free bi-crystals
- No significant effect for the S-Cube bi-crystal since the PSN nuclei are quickly consumed by the migrating S-Cube interface
- Recrystallization kinetics of S-Cube bi-crystal without particle is faster than other bi-crystals with particles
  - S-Cube interface is a special boundary with a nearly 40°<111> misorientation with S

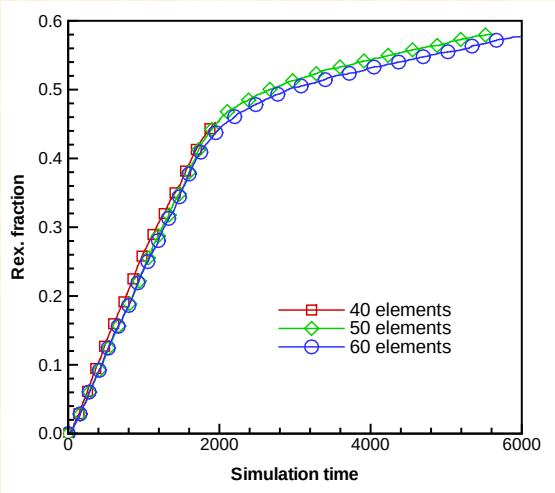
Mesh refinement leads to very minor differences in recrystallization simulations



Cube orientation with spherical particle



S-Cube bi-crystal without particle



S-Cube bi-crystal with spherical particle

- Mesh refinement improves ability to capture gradients in stored energy and orientation, but overall trends remain unaffected
- Recrystallization simulations are not significantly affected by the level of discretization

Summary and Conclusions

- Mesoscale models have been used to study deformation and recrystallization of single crystals and bi-crystals of aluminum
- Deformation simulations capture the non-uniform distributions of stored energy and orientations
  - differences in stored energy across grain boundaries
  - formation of localized deformation zones near hard particles
- Recrystallization simulations capture the evolution of the deformation substructure
  - migration of Cube into S by SIBM
  - formation and growth of nuclei from the deformation zones near particles

Summary and Conclusions (Cont'd)

- Simulations capture micro-growth orientation selection of special nuclei which have 40°<111> misorientation with matrix
- Initial orientation and particle shape influence the nuclei spatial distribution and recrystallization kinetics for single crystals
- Presence of particles at the grain boundary enhances the kinetics and alters the texture for bi-crystals
- Level of mesh refinement did not significantly affect the overall results

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