

# **Coupled Mesoscale Simulations of Hot Deformation and Recrystallization**

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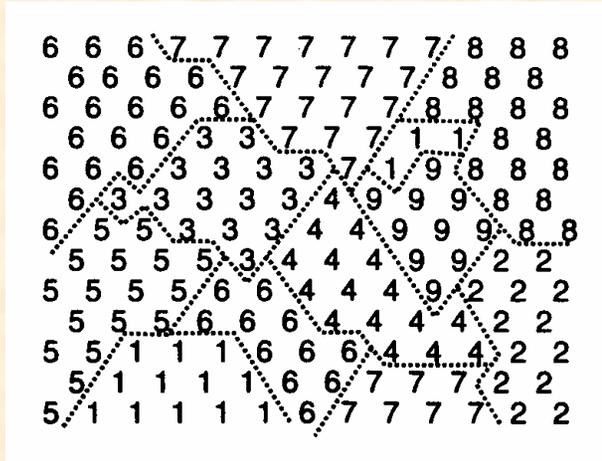
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# Outline

- **Conventional approaches to simulate recrystallization**
- **Novel approach to simulate recrystallization in aluminum**
- **Coupled finite element – Monte Carlo approach**
- **Extraction of deformation substructure from finite element simulations**
- **Recrystallization simulations**
  - **Bicrystals**
  - **bicrystals and tri-crystals with hard particles**
- **Summary and Conclusions**
- **Future Work**

# Traditional Monte Carlo simulation of recrystallization



- Lattice energy consists of bulk stored energy and grain boundary energy
- Sites visited randomly and local energy of site and neighborhood calculated before and after attempted flip
- Flips executed based on probability rules

$$E = \frac{1}{2} \sum_i^n \sum_j^{NN} J(S_i S_j) (1 - \delta_{S_i S_j}) + \sum_i H_i$$

$$p(S_i, S_j, \Delta E, T) = \begin{cases} \frac{J(S_i, S_j) \mu(S_i, S_j)}{J_{\max} \mu_{\max}} & \Delta E \leq 0 \\ \frac{J(S_i, S_j) \mu(S_i, S_j)}{J_{\max} \mu_{\max}} \exp(-\Delta E / kT) & \Delta E > 0 \end{cases}$$

# Boundary energy and mobility depend on misorientation

- **Boundary energy for general boundaries based on Read-Schockley formalism**

$$\gamma = \begin{cases} 0 & \omega = 0 \\ \gamma_0 \frac{\omega}{\omega^*} \left\{ 1 - \ln \left( \frac{\omega}{\omega^*} \right) \right\} & 0 < \omega \leq \omega^* \\ \gamma_0 & \omega > \omega^* \end{cases}$$

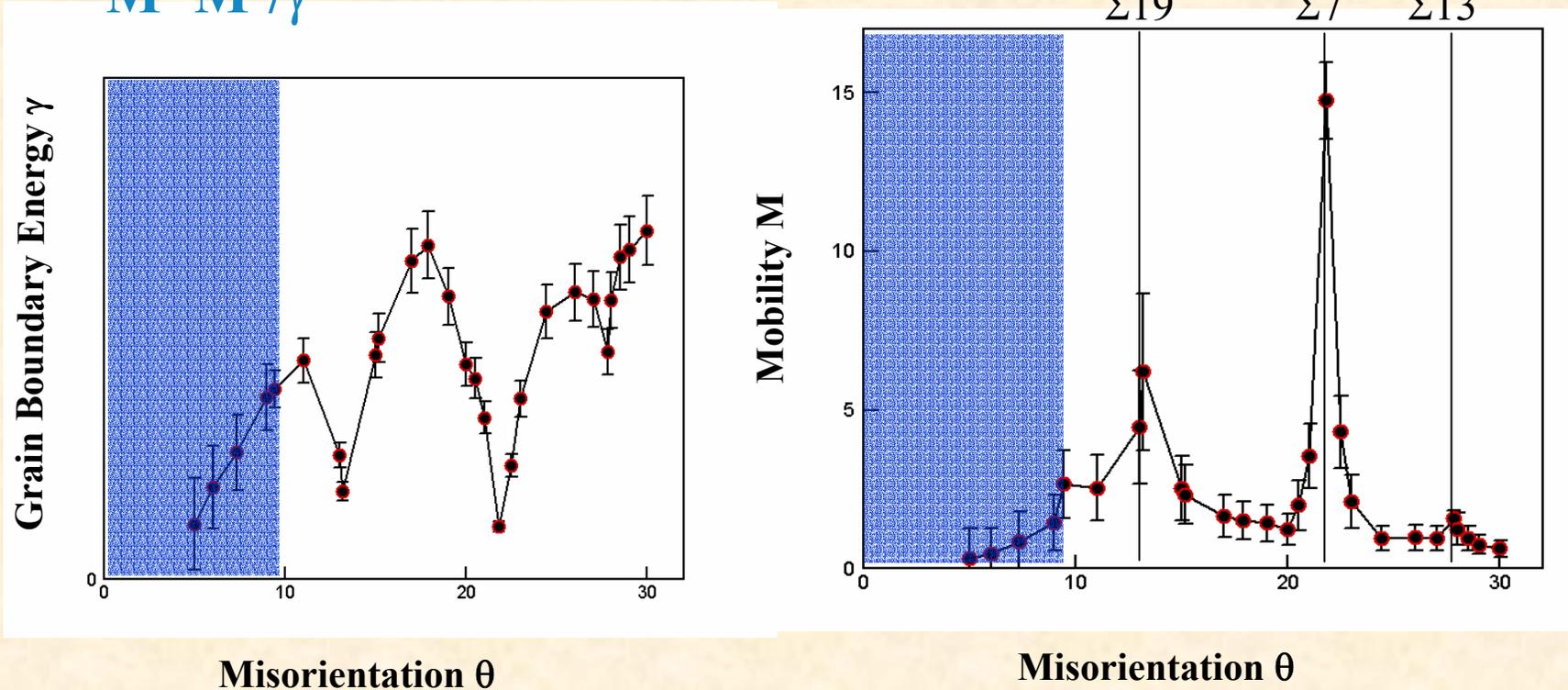
- **Boundary mobility for general boundaries based on empirical equation obtained by fitting to experimental data**

$$\mu = \mu_0 \left[ 1 - \exp \left( -k\omega^n \right) \right]$$

# Energy and mobility of $\Sigma 7$ boundaries obtained from molecular dynamics simulations (Upmanyu et al.)

- Extract boundary energy from total energy vs. half-loop height  
(assume constant entropy)

- $M = M^* / \gamma$



# Traditional mesoscale Monte Carlo models of recrystallization have limitations

- **Models do not incorporate details of deformation substructure**
  - require distinct nucleation and growth phases
  - phenomenological treatment of nucleation
- **Kinetics of evolution not captured accurately for recrystallization and simultaneous grain growth**
  - Models curvature-driven growth
  - Fails to capture linear relationship between driving force and velocity during recrystallization
  - Does not model simultaneous recovery

# Recrystallization in aluminum is due to heterogeneous evolution of deformation substructure

- Deformation substructure depends on temperature, strain rate, stacking fault energy
  - Aluminum, high temperature, low strain rate: obtain well developed cell / subgrain structure
- Recrystallization occurs mainly through discontinuous (abnormal) subgrain growth
- Stored energy of deformation per unit volume can be assumed to be the surface energy per unit volume of subgrain boundaries

$$S_v = 2 / D$$

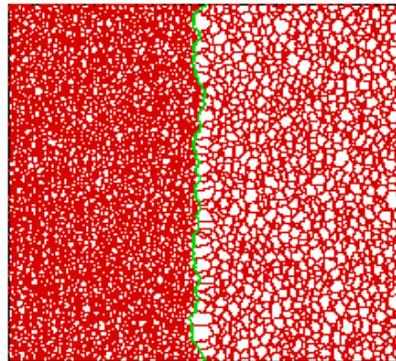
$$H_v = S_v \gamma = \frac{2\gamma}{D}$$

- Interface migration occurs from low-energy into high-energy regions (SIBM nucleation mechanism)

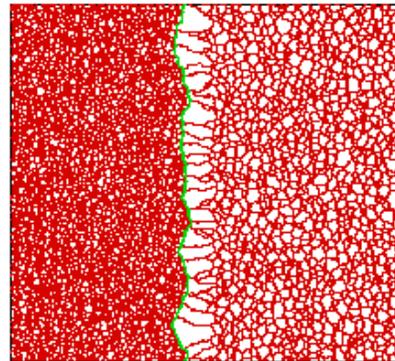
# Proposed approach for simulating recrystallization has several advantages

- Nucleation by SIBM mechanism comes out naturally in the simulations; no need for phenomenological assumptions
- Changes in local driving force due to substructure recovery automatically taken into account
- Local driving forces are only due to boundary energies, no bulk stored energy term, therefore velocity-driving force relationships are captured accurately (no need for hybrid models)

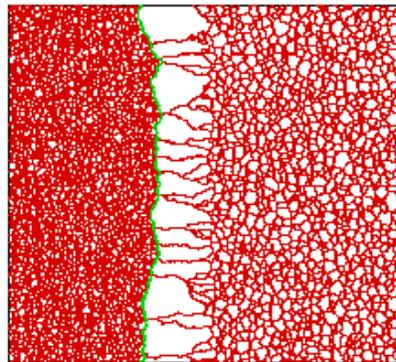
# MC simulation of interface migration driven by difference in stored energy of deformation



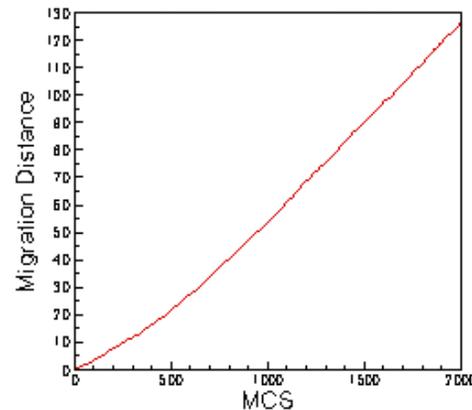
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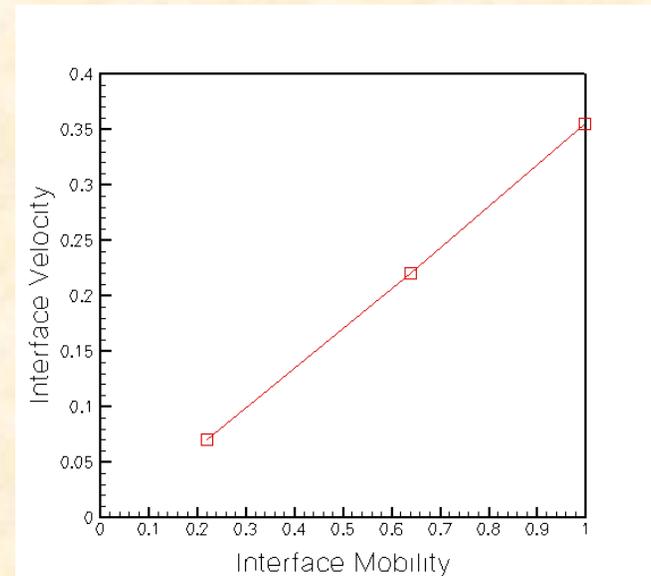
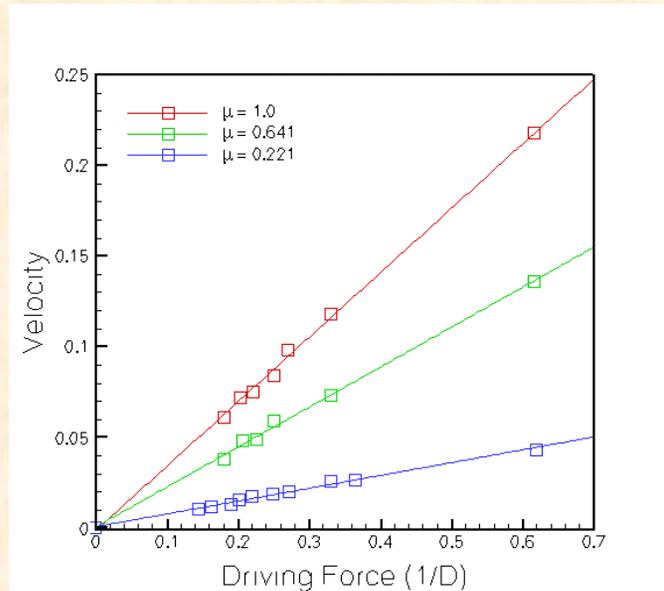


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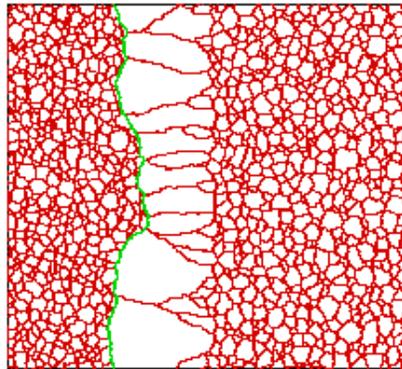
- Interface migrates into region with higher stored energy
- Transient phase where stored energy behind the interface decrease
- When steady-state is reached, interface velocity becomes constant

# Interface velocity varies linearly with driving force, slope proportional to interface mobility

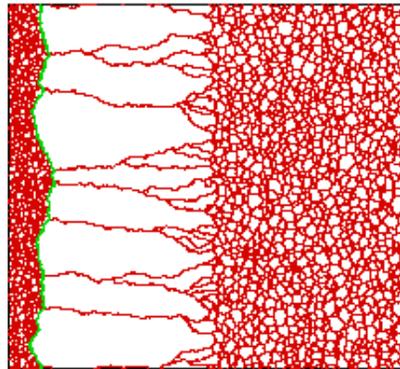


- Variation in driving force obtained by keeping  $\theta$  constant and varying  $D$  across the interface
- Recovery of substructure by subgrain growth suppressed in the bulk  
All straight lines pass through origin
- Slopes proportional to interface mobility

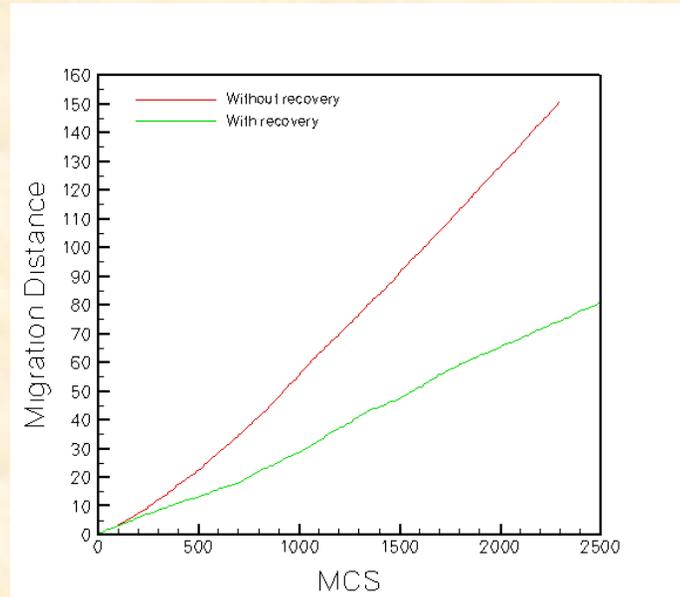
# Recovery of subgrain structure by normal growth can slow down interface migration velocity significantly



With recovery by subgrain growth

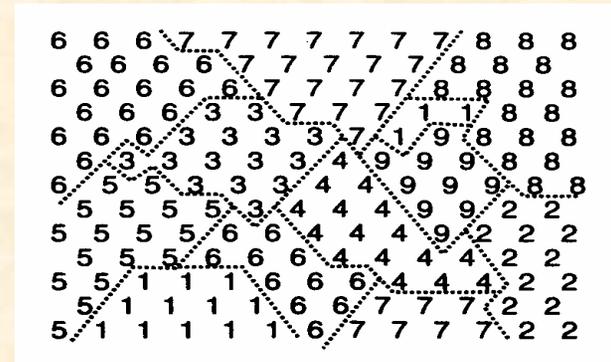
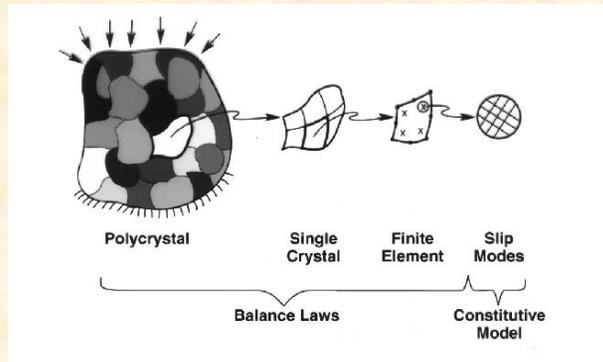


Without recovery



- Recovery by subgrain growth not taken into account in conventional MC simulations
- Becomes more significant at low interface mobilities

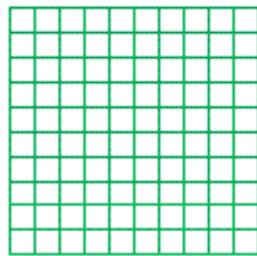
# Approach: coupled finite element - Monte Carlo simulation



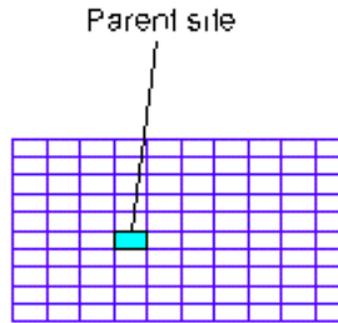
- **Microstructural deformation modeled using finite element technique to capture non-uniform stored energy and orientation distributions**
- **Deformation substructure extracted from FE model and evolved using Monte Carlo technique to capture substructure evolution kinetics, microstructure and texture**
- **Simulations with statistically significant number of grains require the use of massively parallel computing techniques**

# Mapping of information from deformation simulation to Monte Carlo grid

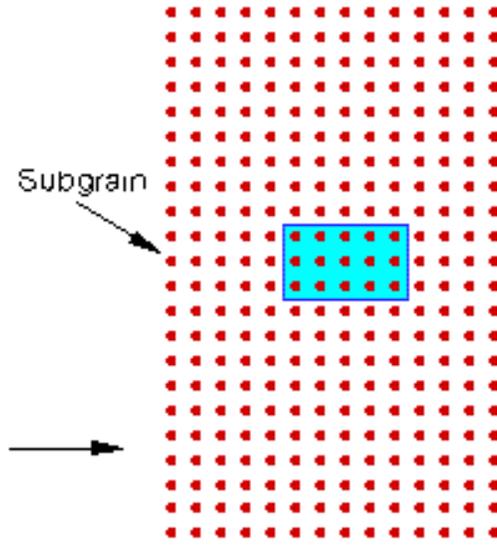
$$H = \frac{\gamma}{2d} \left[ \frac{\Delta\theta}{\theta^*} \left( 1 - \ln \frac{\Delta\theta}{\theta^*} \right) \right]$$



(a) Initial mesh



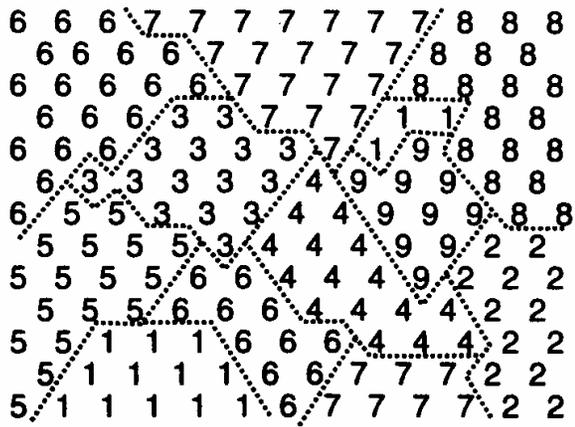
(b) Deformed mesh



(c) Monte Carlo grid

- Each parent site contains axis and angle  $\theta$  and stored energy  $H$
- Each subgrain site is associated with
  - mean subgrain size  $d$
  - mean misorientation between subgrains  $\Delta\theta$  (about  $\theta$ )

# Monte Carlo simulation of substructure evolution – recrystallization by abnormal subgrain growth



- **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 described by misorientation between boundary sites

$$E = \frac{1}{2} \sum_i^n \sum_j^{NN} J(S_i S_j) (1 - \delta_{S_i S_j})$$

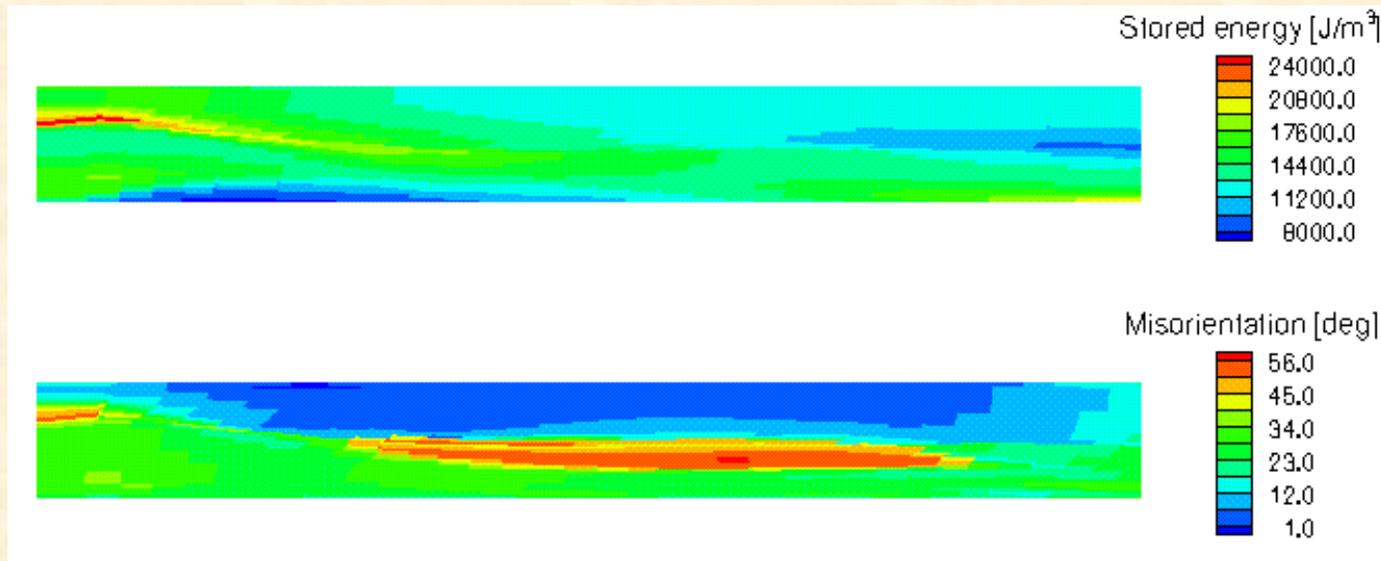
$$N_{MCS}^{\mu\gamma} = N_{MCS} \frac{\mu\gamma}{\mu_{max}\gamma_{max}}$$

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

# Simulations

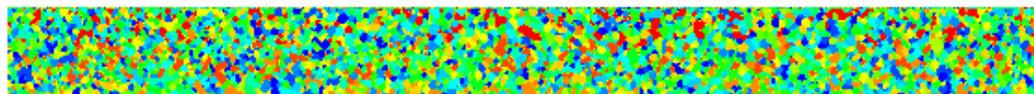
- **Recrystallization of aluminum aluminum bicrystals after hot deformation**
  - SIBM mechanisms at the boundary between various known deformation texture components
  - Origin of cube texture evolution during recrystallization
- **Bicrystals and tri-crystals containing non-deformable particles**
  - Origin of “random” texture components
  - Comparison recrystallization kinetics due to hard particles and grain boundary nucleation

# Deformation of brass-S bicrystals: simulation of stored energy and orientation distributions

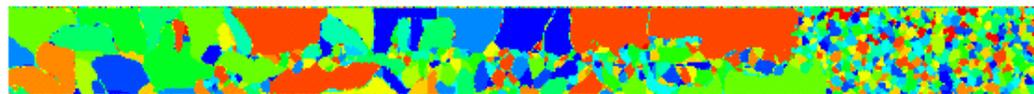


- Lower stored energy in brass compared to S
- Large misorientations in brass and S near the interface

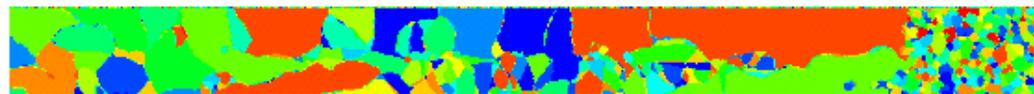
# Simulating the recrystallization of brass-S bicrystal by abnormal subgrain growth



MCS = 0



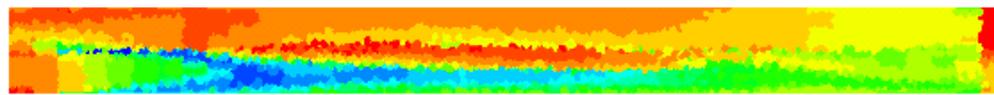
MCS = 500



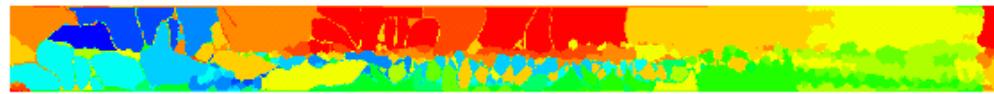
MCS = 1000

- Color scheme represents grain number
- Initial subgrain size in deformation substructure uniform across brass and S

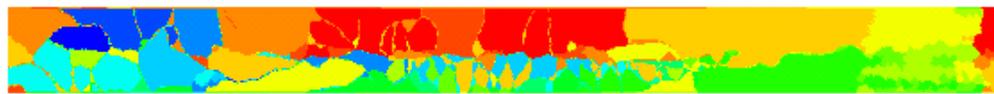
- Color scheme represents rotation angle, blue near-cube
- Rotated-cube orientations at interface grow abnormally, strengthening component after recrystallization



MCS = 0

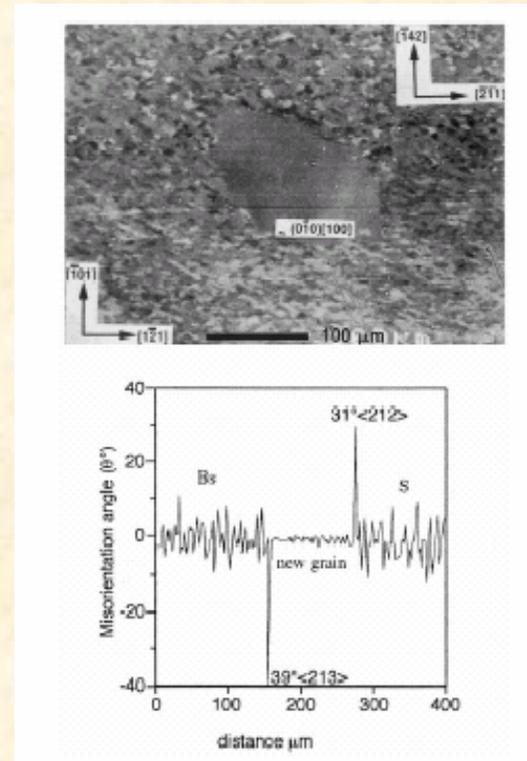
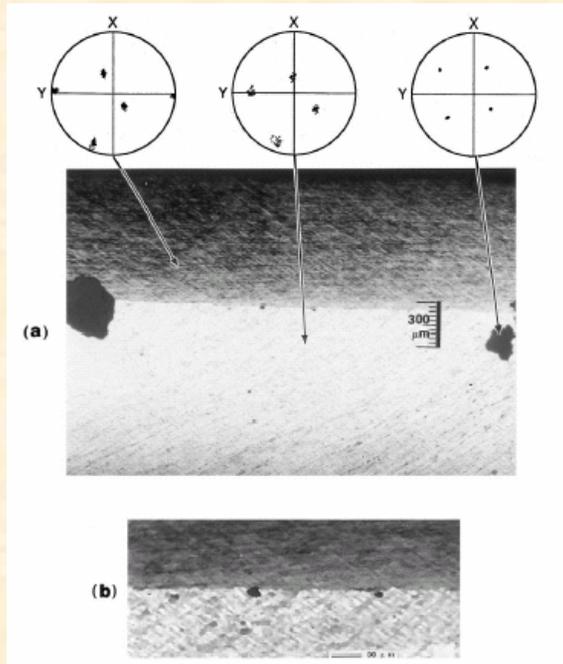


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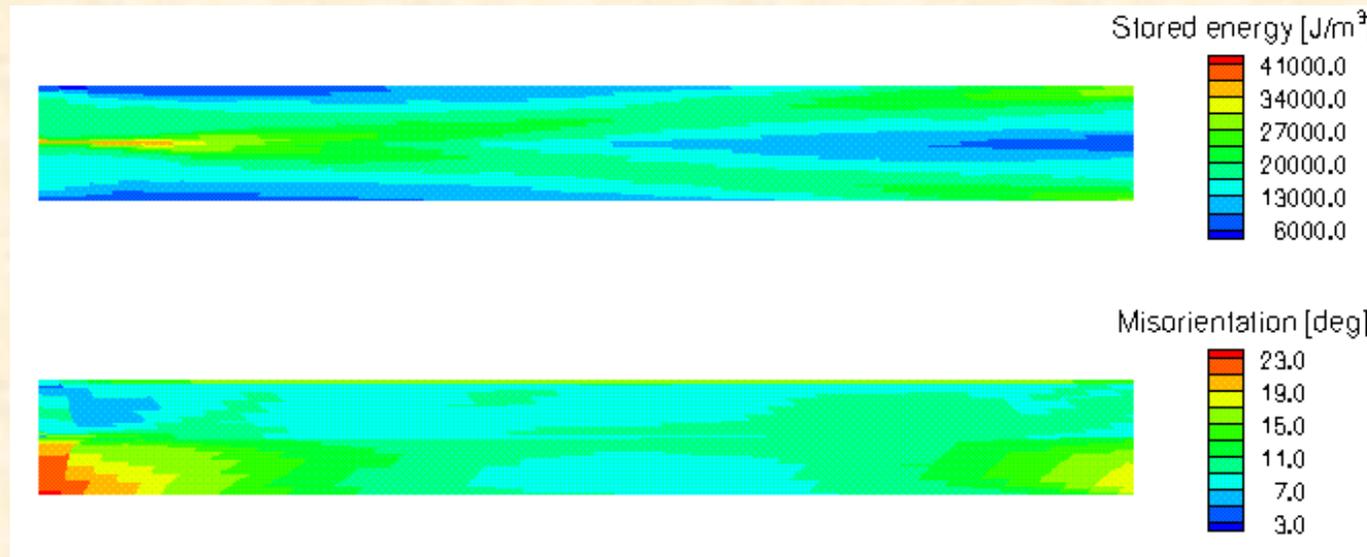
MCS = 1000

# Deformation and recrystallization of brass-S bicrystals: experimental Data



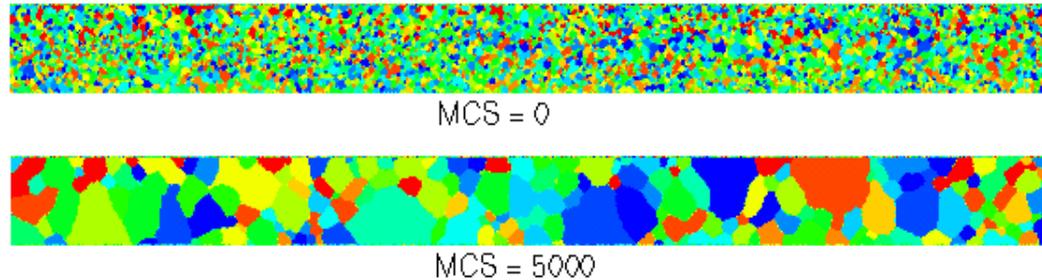
- Nucleation and growth of near-cube grains at the interface

# Deformation of copper-S bicrystals: simulation of stored energy and orientation distributions



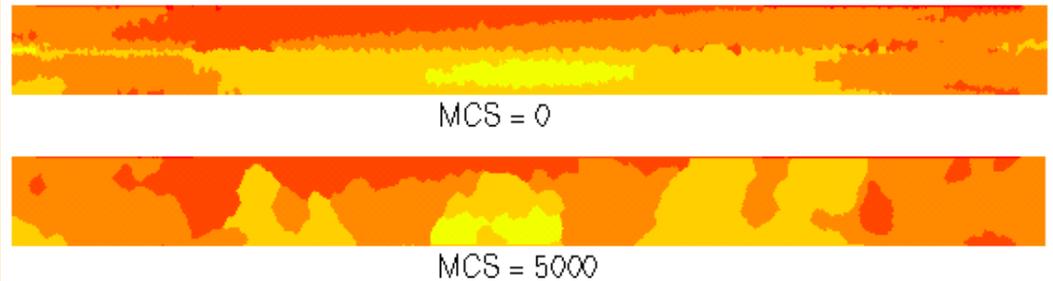
- Roughly same stored energy in copper and S
- Formation of high misorientation in certain areas

# Simulating the recrystallization of copper-S bicrystal by abnormal subgrain growth

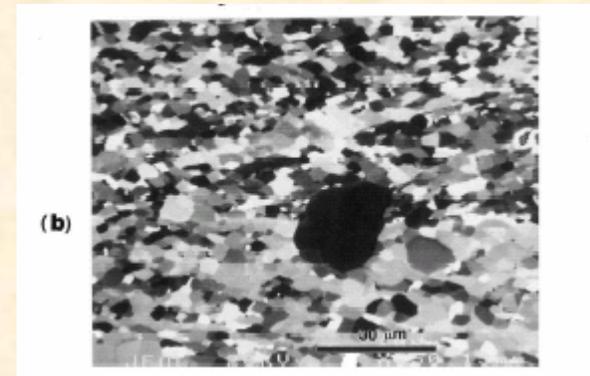
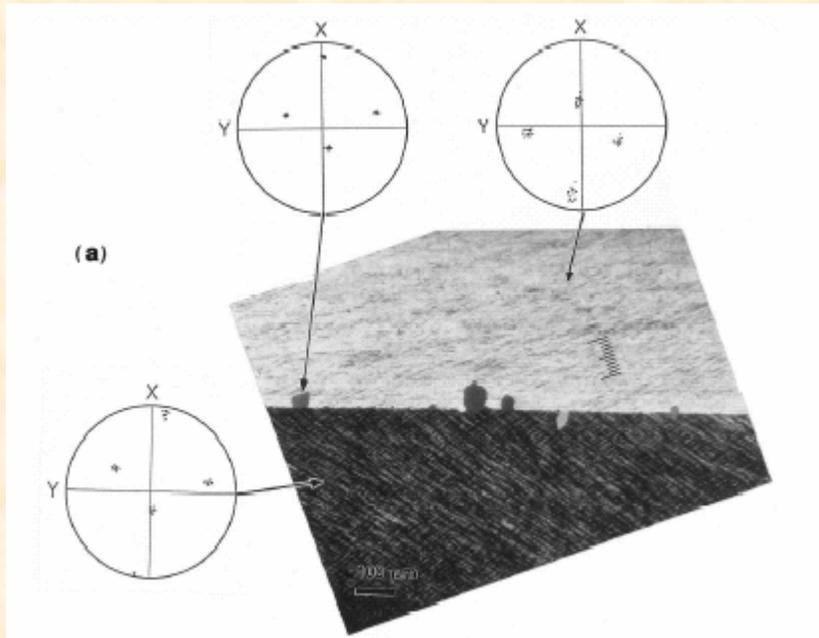


- Deformation substructure uniform across copper and S
- Grain structure more uniform after recrystallization than in brass-S bicrystal

- Formation of nuclei at the interface and growth in either
- No significant change in texture

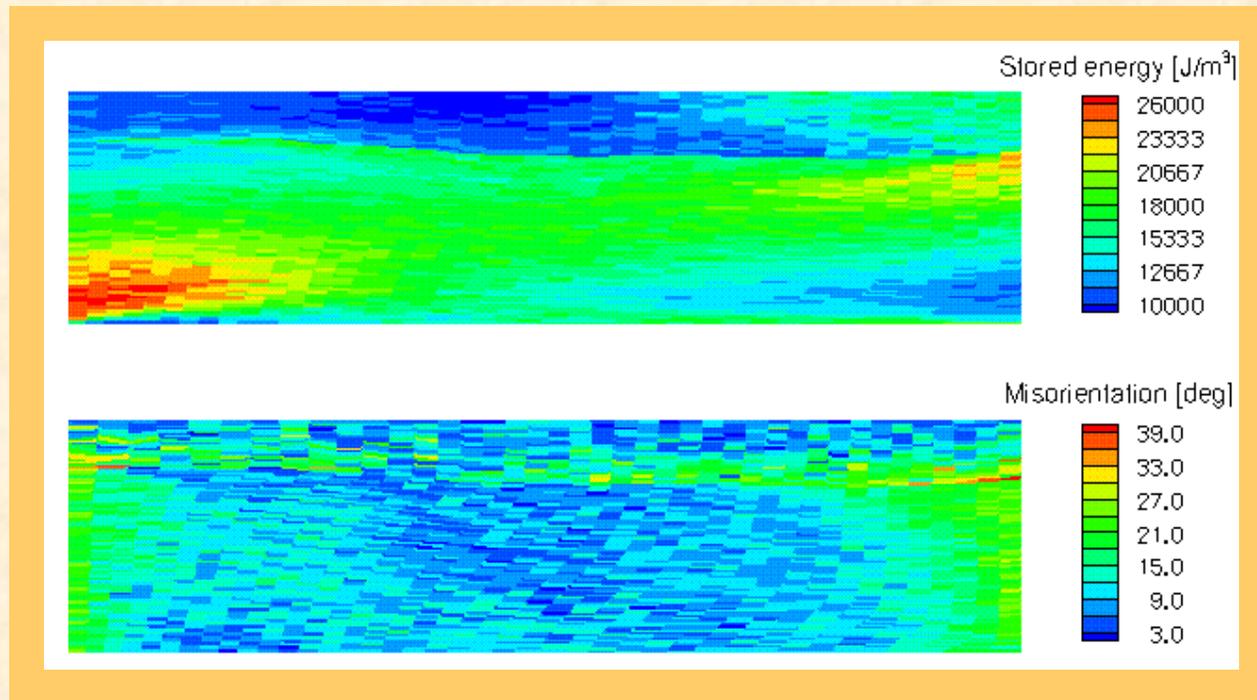


# Deformation of copper-S bicrystals: experimental Data



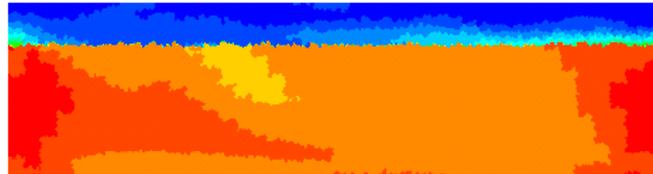
- **SIGM based nucleation of grains not much misoriented from either copper or S**

# Simulating the hot deformation of cube-S bicrystal

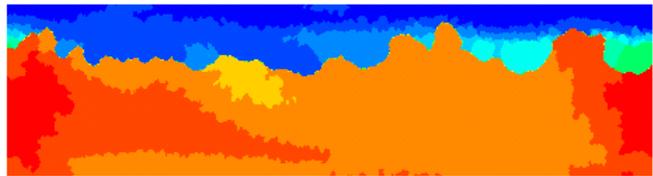


- Lower stored energy in cube than in S
- Low misorientations within the bulk of cube and S
- Larger misorientations in cube and S at the interface

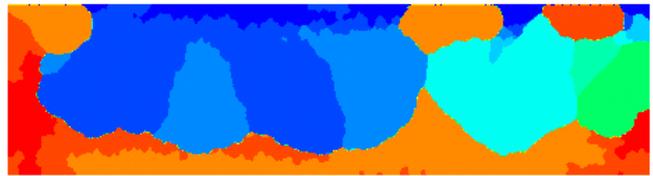
# Simulating the recrystallization of cube-S bicrystal by abnormal subgrain growth



MCS = 0

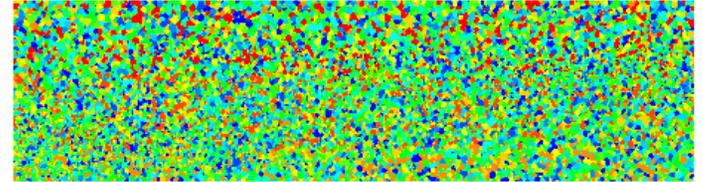


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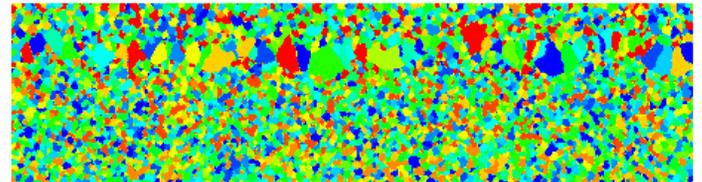


MCS = 5000

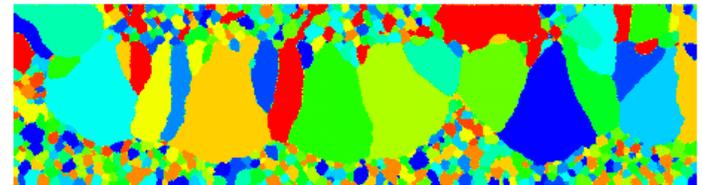
- Initial  $\Sigma 7$  boundaries rotated out of Brandon's criterion after deformation
- Many cube grains grow into S, some at angle to elongation axis



MCS = 0



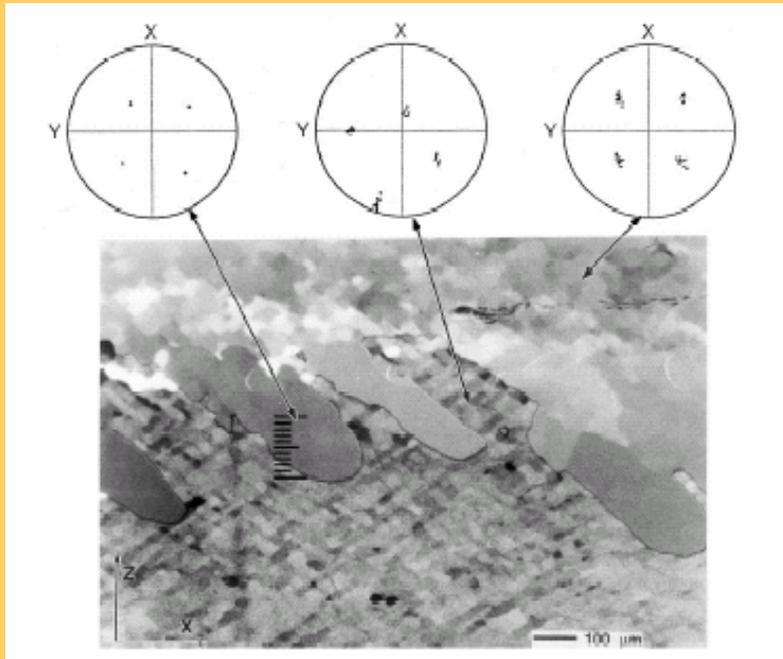
MCS = 1000



MCS = 5000

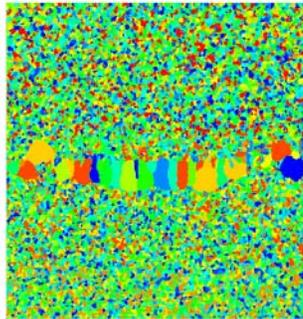
- Initial subgrain size within the cube is larger compared to that in S, indicating lower stored energy within cube

# Deformation and recrystallization of cube-S bicrystals: experimental Data

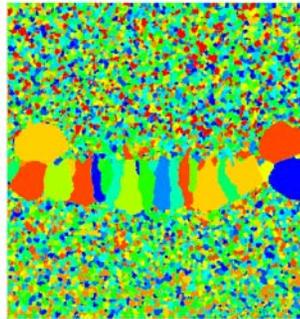


- Lower stored energy in cube compared to S
- Cube grains grow into S at an angle
- Special boundary ( $\Sigma 7$ ) at the tip of growing cube
- Twist boundary with low mobility at the sides
- Deformation at 400C, strain rate 0.1/s,  $e=-1.4$

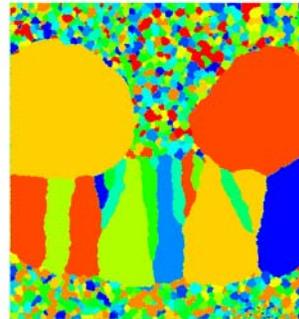
# Effect of particle on recrystallization – bicrystal study



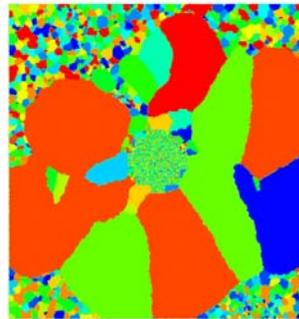
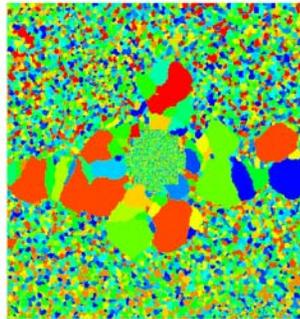
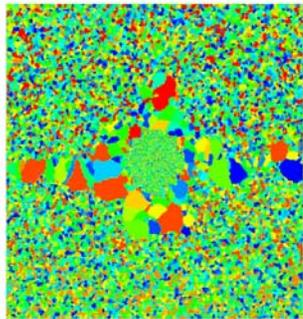
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MCS = 1000



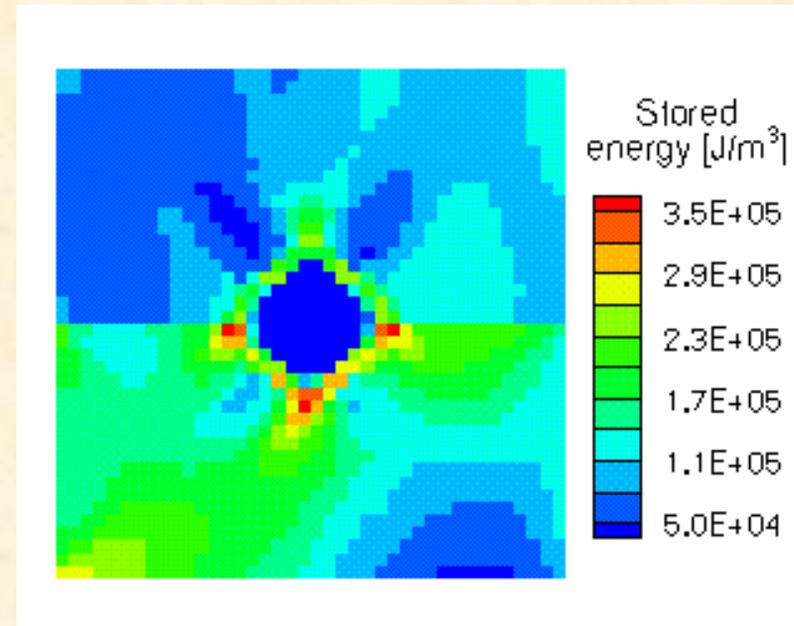
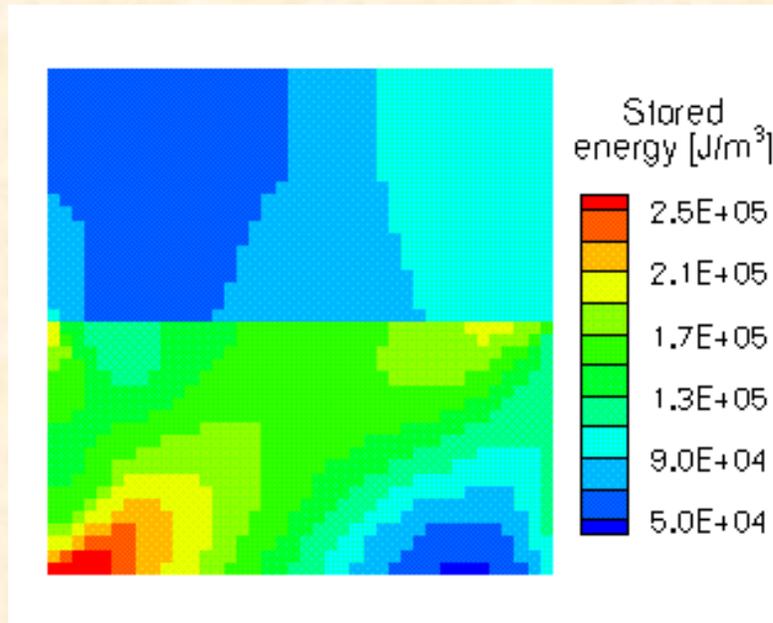
MCS = 4000



Recrystallization of a cube-S bicrystal (top) and a cube-S bicrystal with a non-deformable particle in the grain boundary hot-deformed 50% in plane strain compression

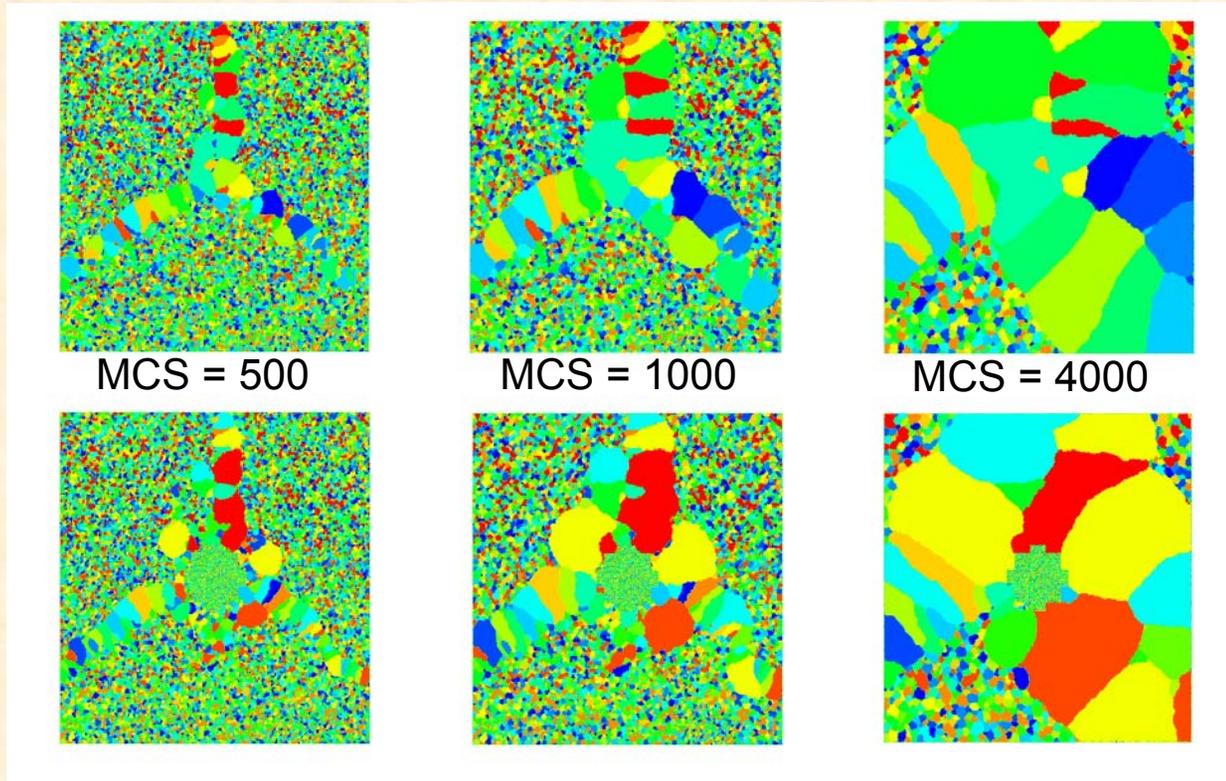
- Bi-crystal consists of cube on top and S in the bottom
- In the absence of hard particle, cube grain migrates into S strengthening cube texture during recrystallization
- In the presence of hard particle in the grain boundary, abnormal growth fronts nucleated at the particle grow in both S and cube grains
- Origin of “random” texture development during recrystallization in particle-containing Al alloys

# Comparison of stored energy distributions with and without hard particle: cube-S bicrystal study



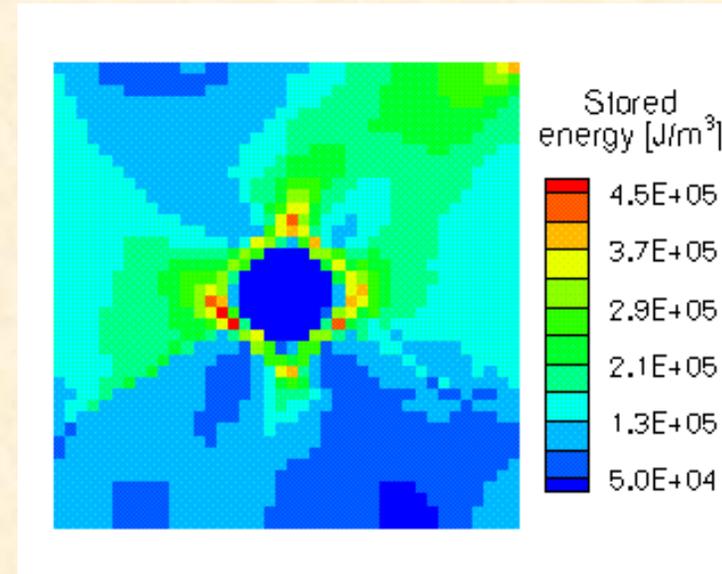
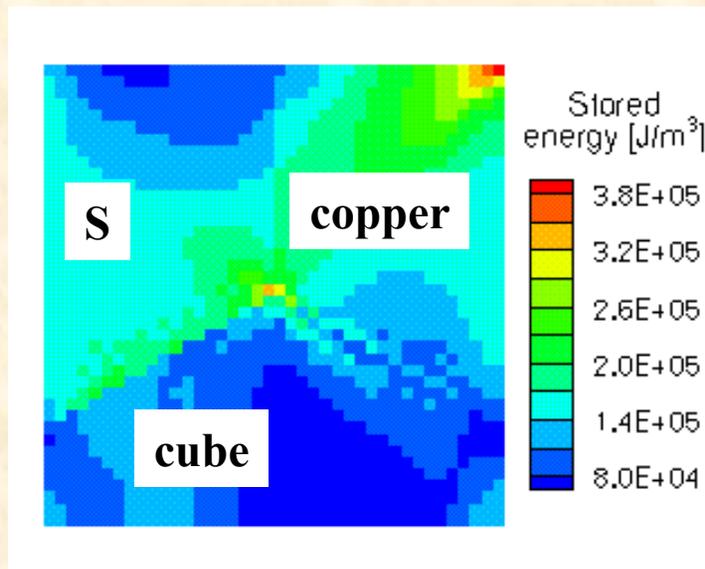
- Localized high stored energy regions are formed near the hard particles, especially in the S grain and S-cube interface

# Effect of particle on recrystallization: tri-crystal study



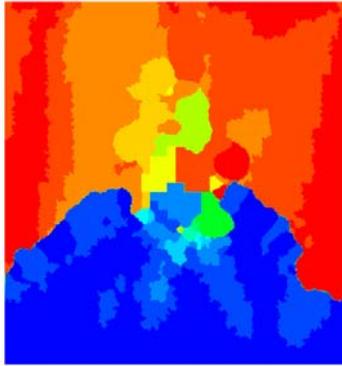
- In the presence of a hard particle at the triple point, the nucleation pattern does not deviate significantly from the case where there is no hard particle, although the average recrystallized grain size is bigger in the presence of hard particle

# Comparison of stored energy distributions with and without hard particle: cube-S-copper tri-crystal study



- Localized high stored energy regions near hard particle are formed especially in the copper and S grains

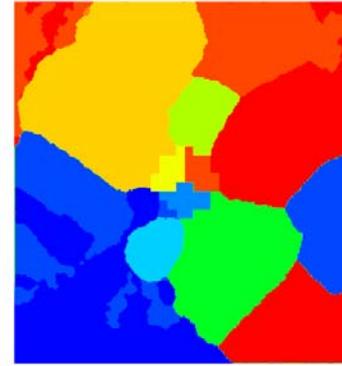
# Formation of “random” texture: tri-crystal



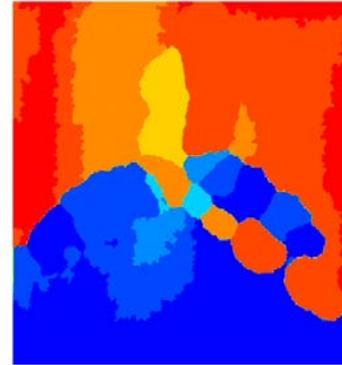
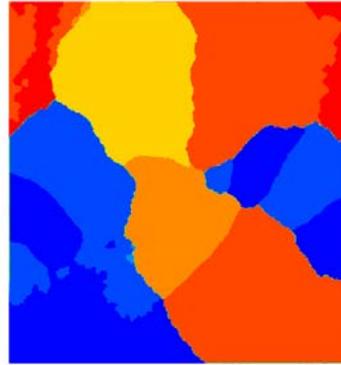
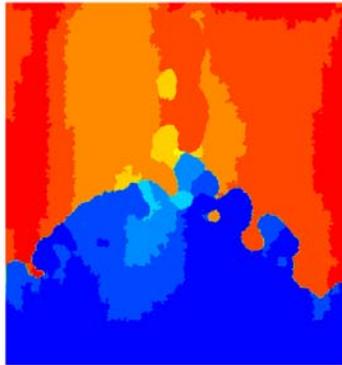
MCS = 500



MCS = 1000

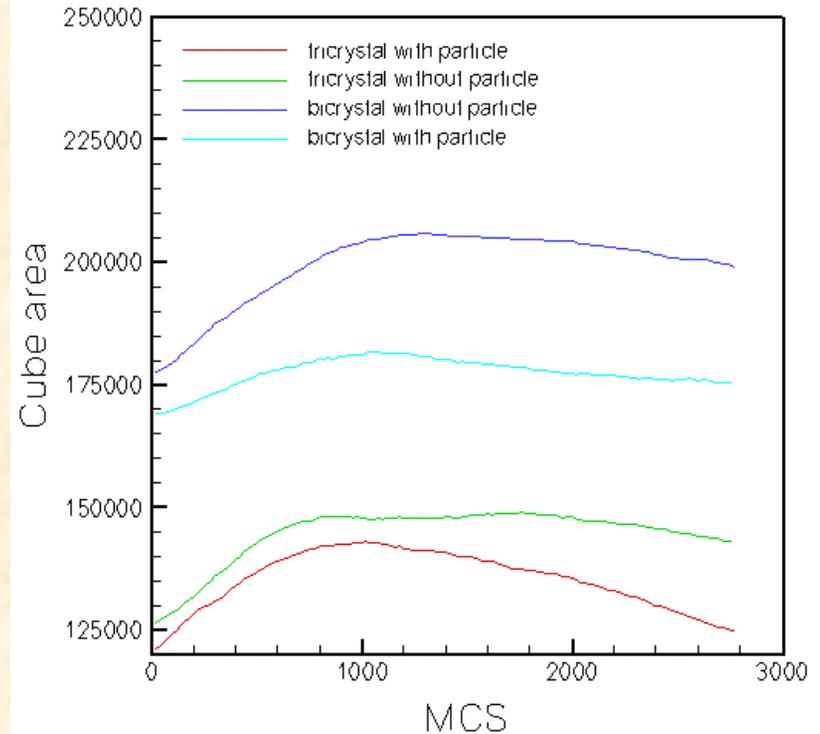
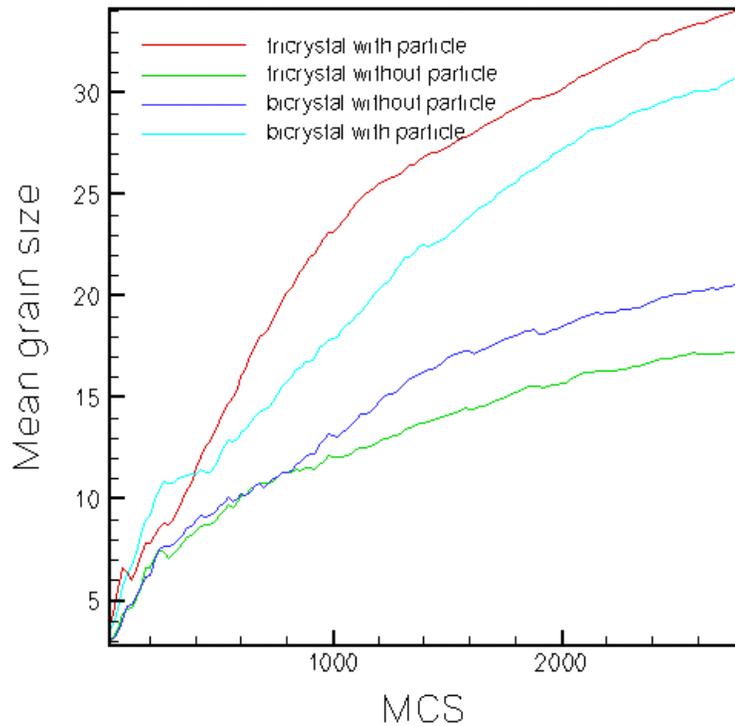


MCS = 4000



- In the presence of a hard particle at the triple point, the orientations of grains that nucleate and grow are different. Grains of significantly new orientation (colored green) seen to grow in the presence of hard particle

# Subgrain growth kinetics is influenced by hard particles



- Subgrains grow faster in the presence of hard particles
- Area fraction of cube orientation decreases in the presence of hard particles

# Summary

- **Recrystallization of hot-deformed aluminum was simulated by treating it as an abnormal subgrain growth process using a Monte Carlo approach**
- **The heterogeneous subgrain structure resulting from hot deformation was obtained from finite element simulations of microstructural deformation using crystal plasticity approach**
- **The coupled finite element – Monte Carlo simulation technique was used to study the recrystallization behavior of hot deformed bicrystals and tri-crystals of aluminum with and without non-deformable particles**
- **Simulations correctly reproduced the velocity-driving force relationships of interfaces driven by stored energy differences**
- **Bicrystal studies capture the general trends observed experimentally, although some of the specific aspects of cube growth morphology are not captured**
- **The effect of hard particles in the production of “random” recrystallization texture components, and on the recrystallization kinetics are captured by the model**