Atomistic modeling of grain boundary motion and rotation

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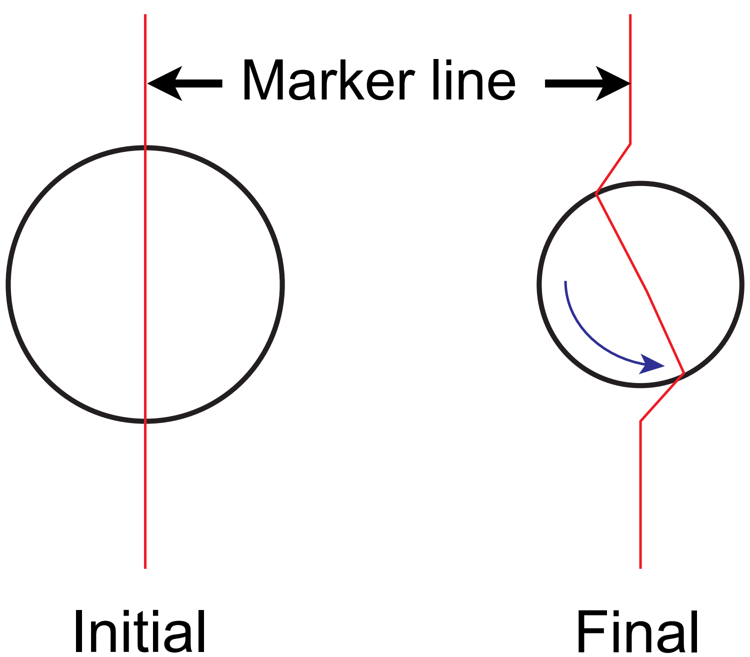
Outline

- Grain rotation was observed experimentally during grain growth and plastic deformation of nano-crystalline materials. It is part of microstructure evolution and must be understood for microstructure control in materials.
- There are open questions related to driving forces of grain rotation and its relation to GB motion, GB sliding and other processes.

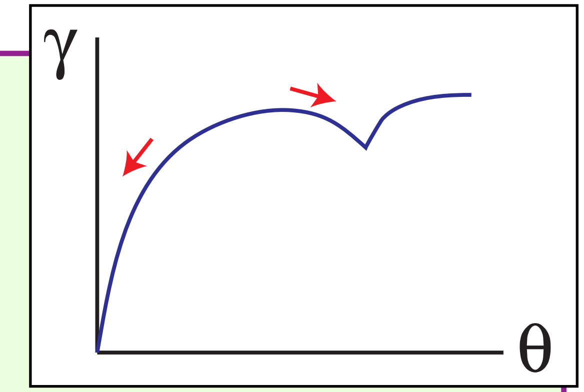
- **This talk will present:**
  - MD simulations for shrinkage, growth and rotation of an isolated grain in copper
  - Dislocation mechanisms explaining the grain behavior
  - Relevance to materials processes

Shrinkage and rotation of a cylindrical grain

We study an isolated cylindrical grain to eliminate the effect of triple lines and other constraints and focus on the rotation process



Driving forces for rotation

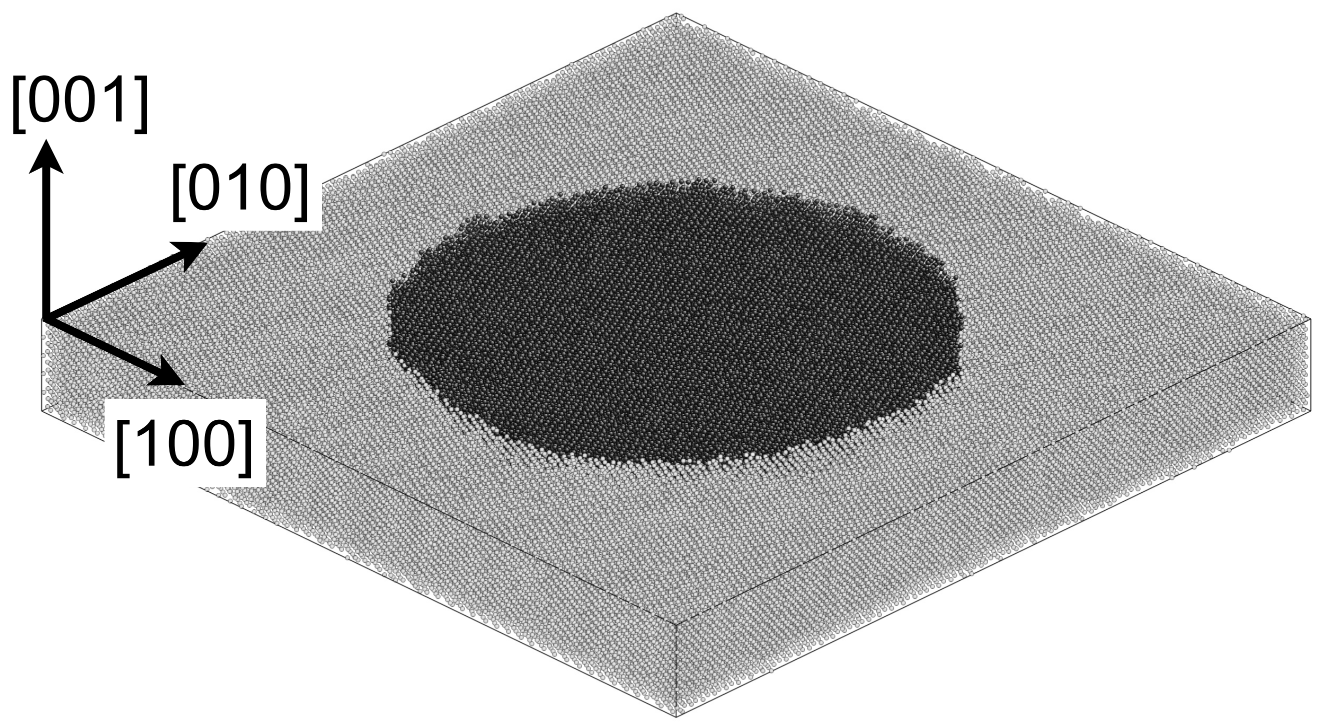


- Applied torque
- Decrease in GB free energy γ
- Coupling effect: GB motion produces shear deformation
  - The grain shrinks due to capillary forces
  - If the GB motion is coupled to shear deformation, the grain must rotate (Cahn and Taylor, 2004)
  - For low-angle GBs the rotation can be easily understood from the conservation of the dislocation content and the Frank relation $\theta \approx b/L$. Thus θ must increase during shrinkage.
  - The coupling competes with decrease in θ due to $\gamma' < 0$ but can win leading increase of θ during shrinkage.

Rotation towards larger θ was observed in MD simulations by Srinivasan and Cahn (2002)

Methodology of simulations

- NPT MD with an EAM potential for Cu. T_m = 1327 K (experimental 1356 K)
- Temperatures 500 - 1350 K
- A specially designed thermodynamic integration procedure to create initial configuration with near-equilibrium GB structure and free volume
- Special procedure for tracking the grain misorientation θ and area $A = \pi R^2$.

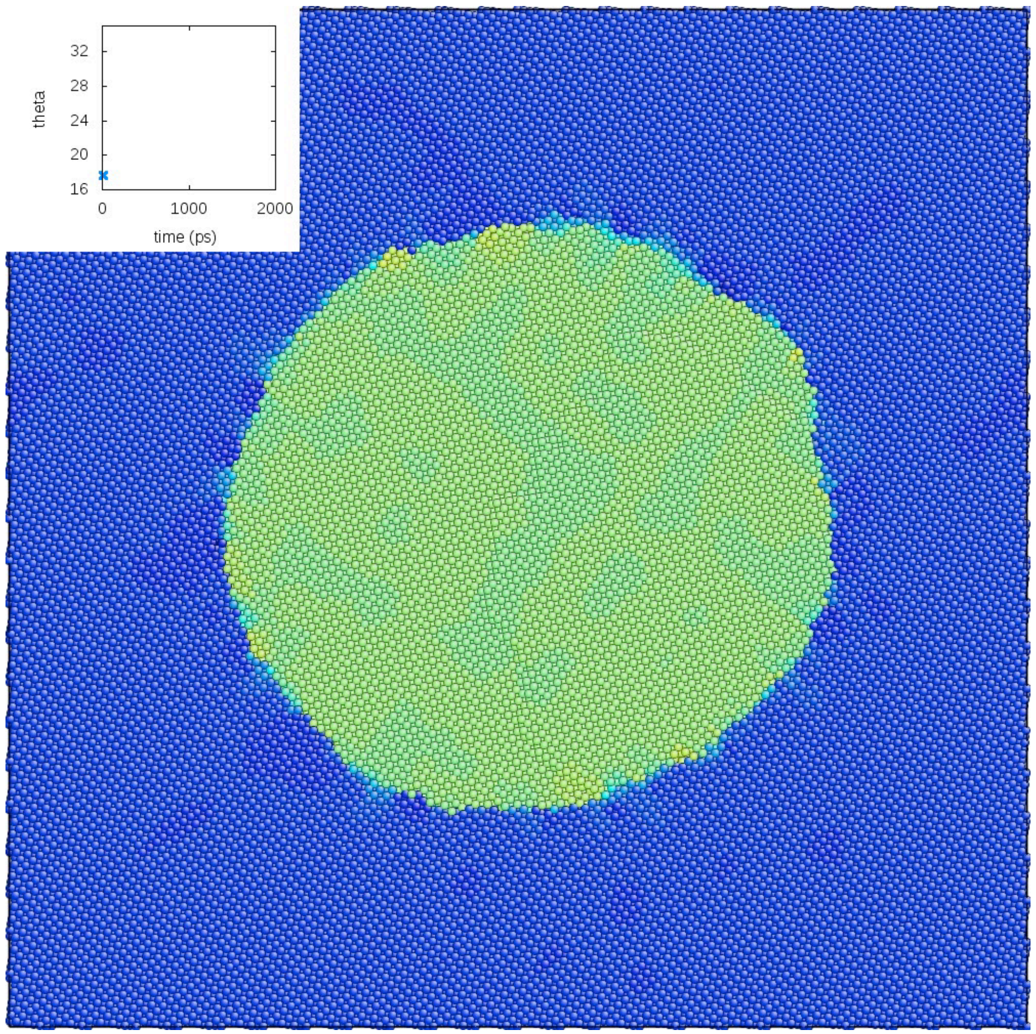


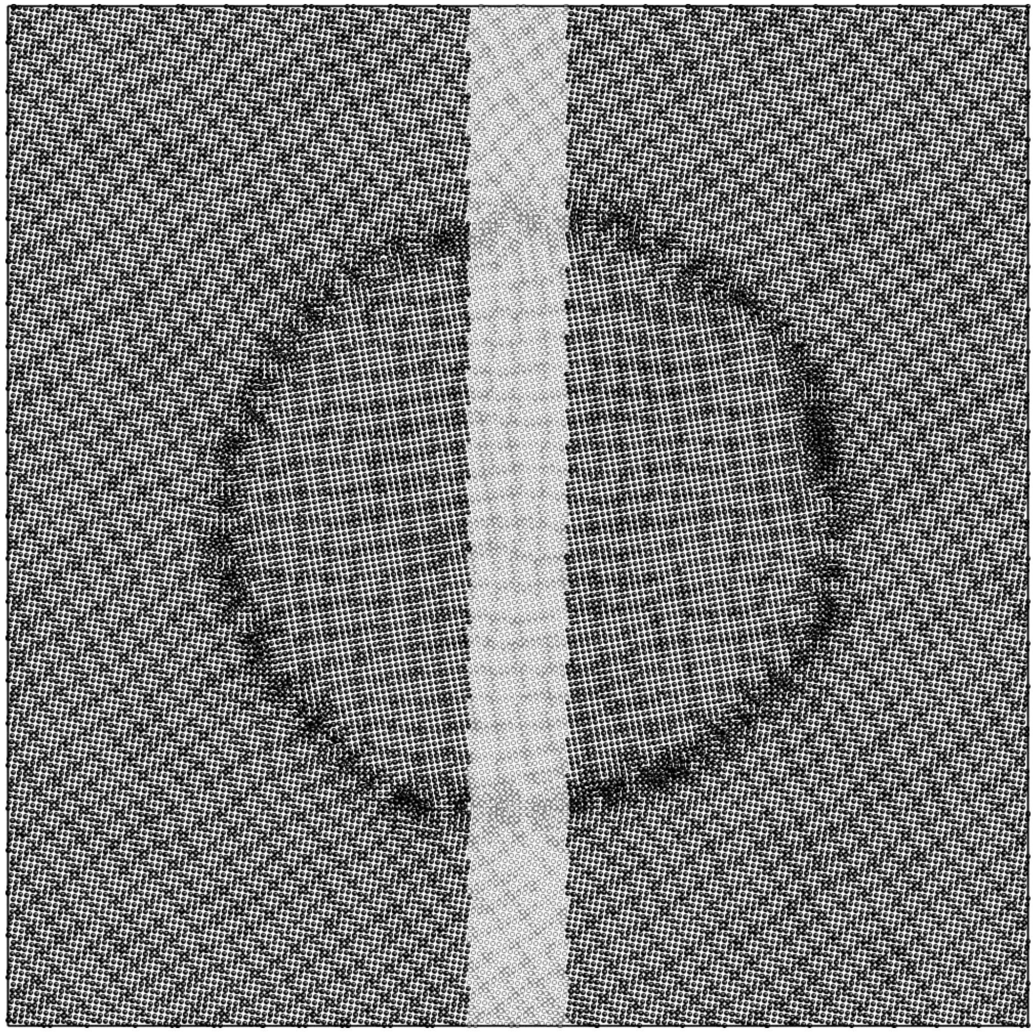
Simulation block

300 x 300 x 36 Å^3

Example of grain shrinkage and rotation

With increasing misorientation





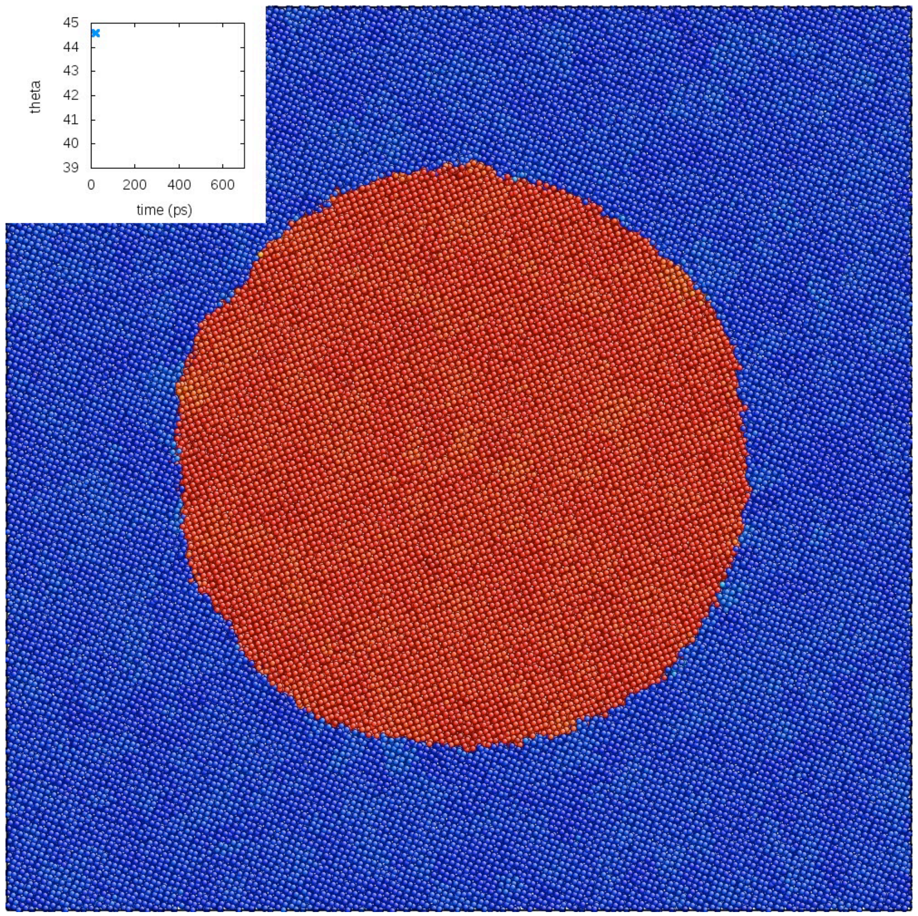
θ = 16.3°; T = 900 K

Capillary driven grain shrinkage produces:

- Grain rotation with increasing θ
- Shear deformation of the surrounding grain (signature of coupling)

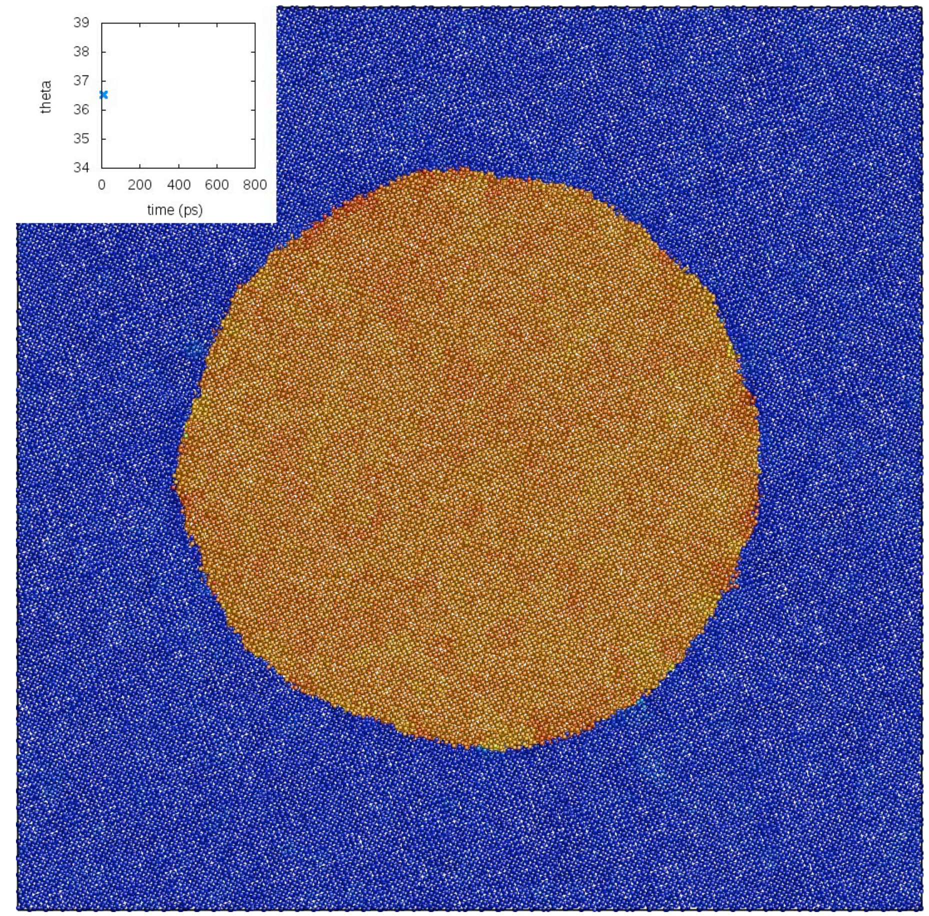
Example of grain shrinkage and rotation

Rotation with decreasing θ



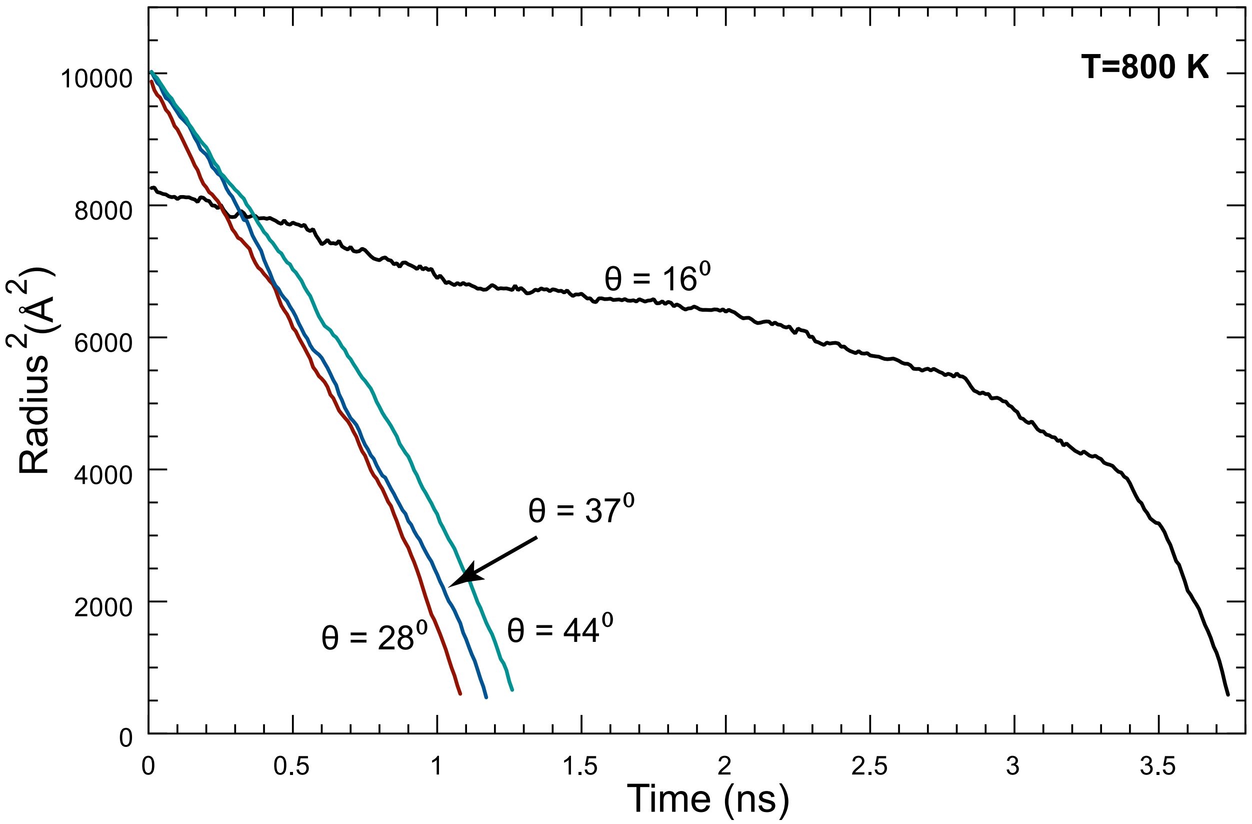
θ = 45.0º; T = 900 K

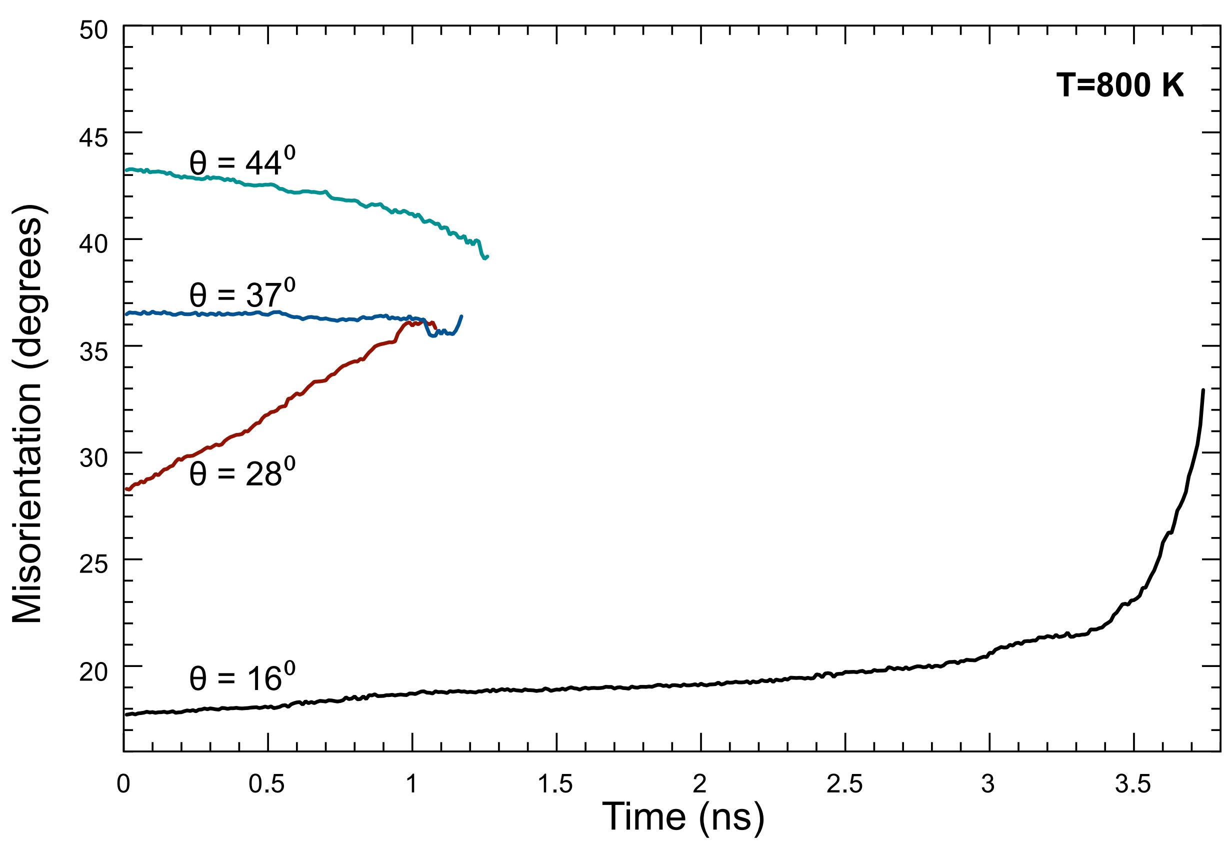
Little rotation



θ = 36.9º; T = 900 K

Grain shrinkage at low temperatures ($0.6T_m$)

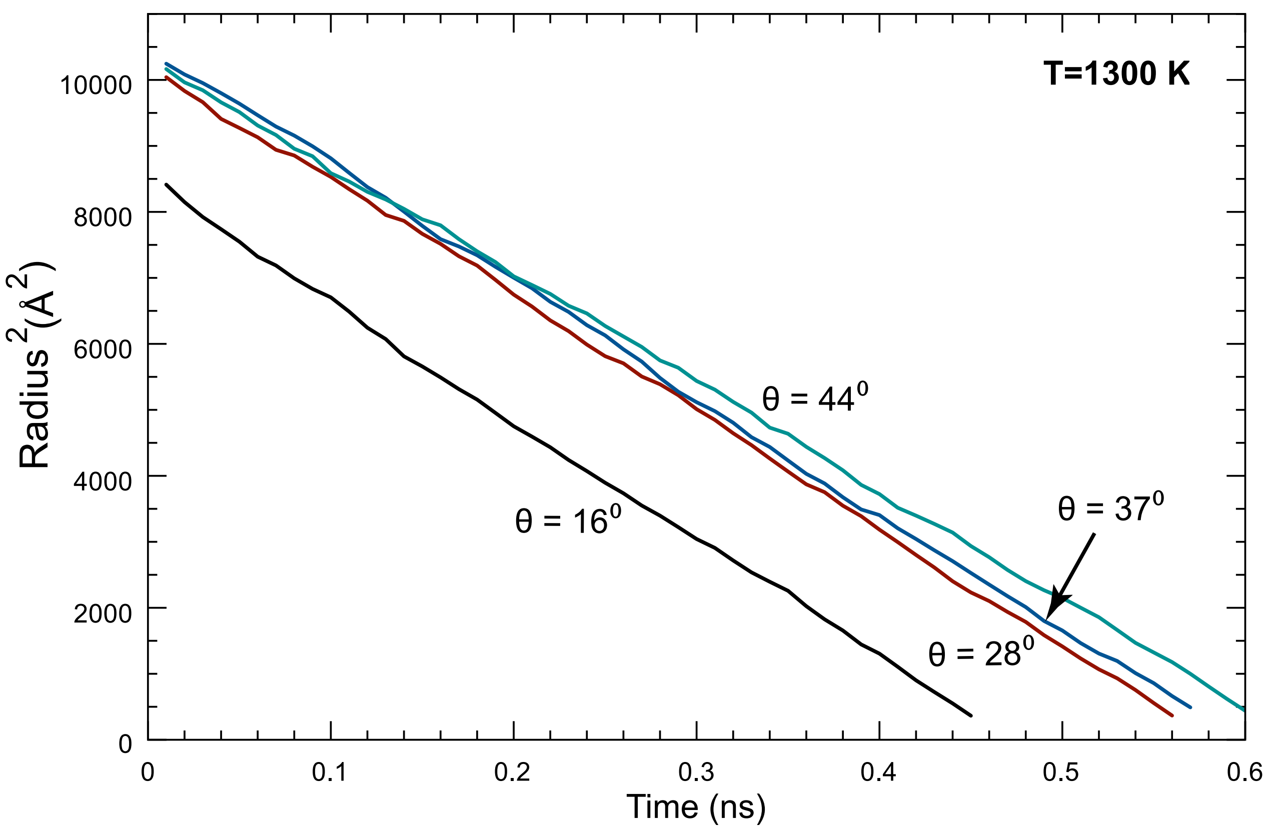


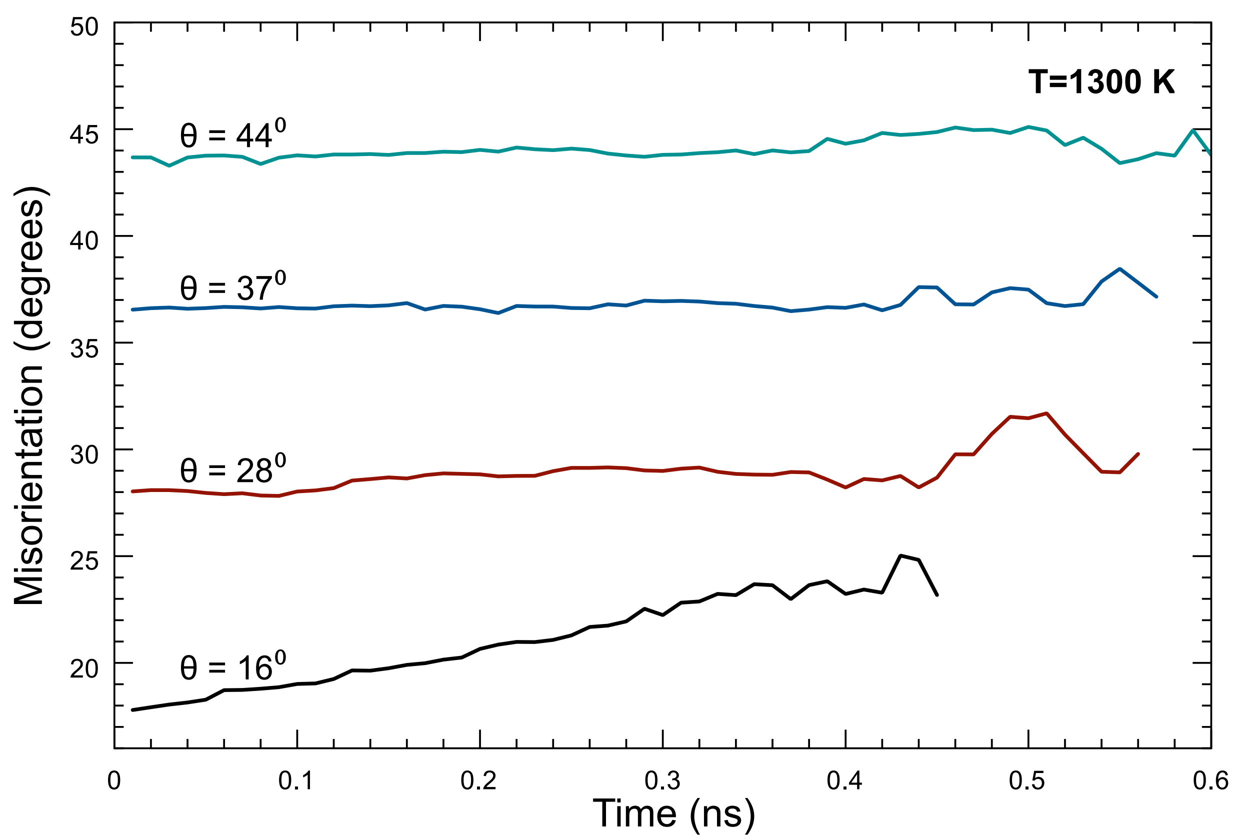


- Low-angle GBs rotate to increase their θ. Indication of coupling
- The θ = 37^o GB does not rotate (almost). Coupling disappears?
- GBs with θ > 37^o rotate to decrease their θ. Negative coupling?
- There is something special about the 35^o to 37^o angles

Similar to Srinivasan and Cahn (2002)

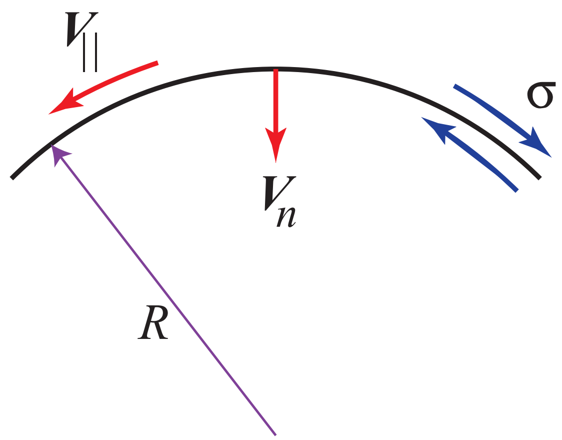
Grain shrinkage at high temperatures ($0.98T_m$)





- Rotation of high-angle GBs ceases, indicating that coupling disappears
- The $\theta = 16^o$ GB still rotates and is partially coupled
- The shrinkage accurately follows the $R^2 \propto$ time law

Cahn-Taylor model of a cylindrical grain (2004)



Coupling-sliding law: $V_{\parallel} = \beta V_n + V_s$

β(θ) - coupling factor; V_s - sliding velocity

Dynamic equations:

$$V_n = M_n\left(\beta\sigma + \frac{\gamma - \beta\gamma'}{R}\right)$$

$$V_{\parallel} = M_n\beta\left(\beta\sigma + \frac{\gamma - \beta\gamma'}{R}\right) + M_s\left(\sigma - \frac{\gamma'}{R}\right)$$

$$\Rightarrow\quad -\frac{d\theta}{d\ln R} = \beta + \frac{M_s\left(\sigma - \frac{\gamma'}{R}\right)}{M_n\left(\beta\sigma + \frac{\gamma - \beta\gamma'}{R}\right)}$$

M_n - mobility coefficient for normal motion; M_s - mobility coefficient for sliding

Limiting case 1: σ = 0 (no applied shear stress) and β = 0 (no coupling)

$$V_n = M_n\frac{\gamma}{R} \quad\Rightarrow\quad R^2 = R_0^2 - 2M_n\gamma t$$

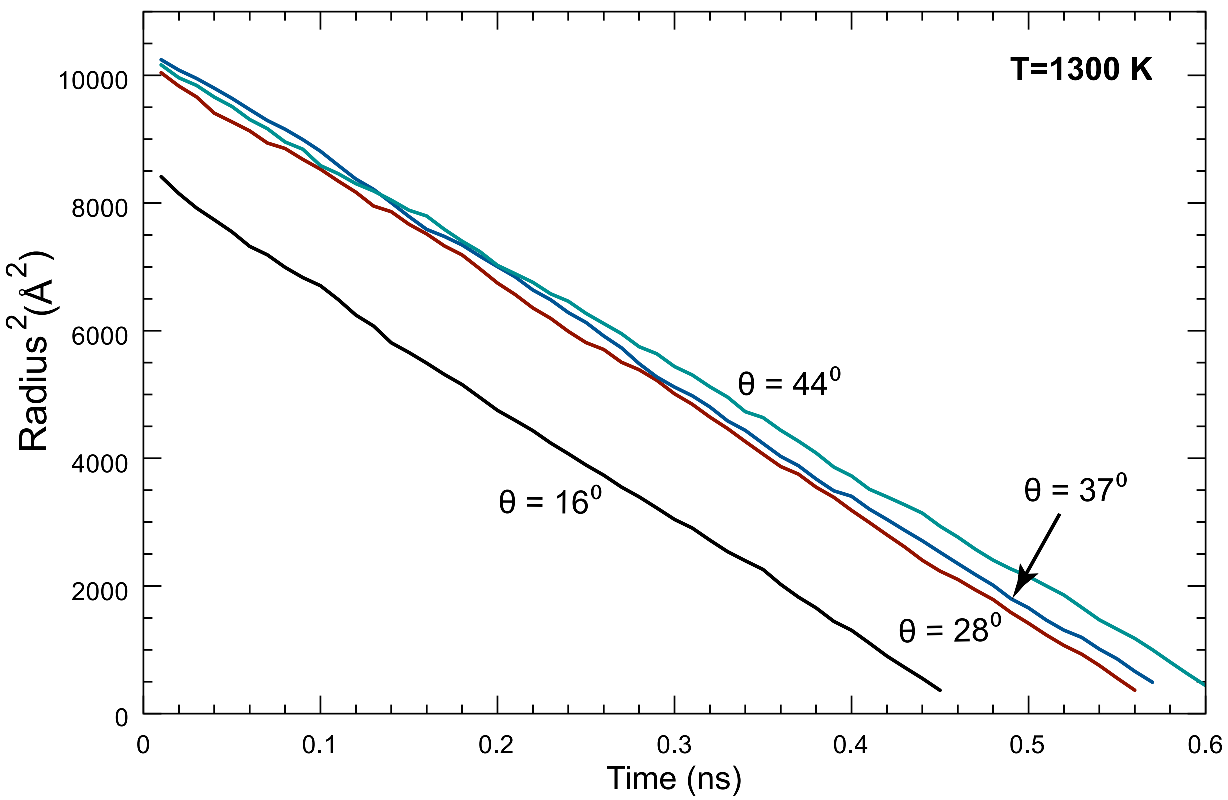
(Parabolic law)

Assuming that M_n is constant

Test of the parabolic law

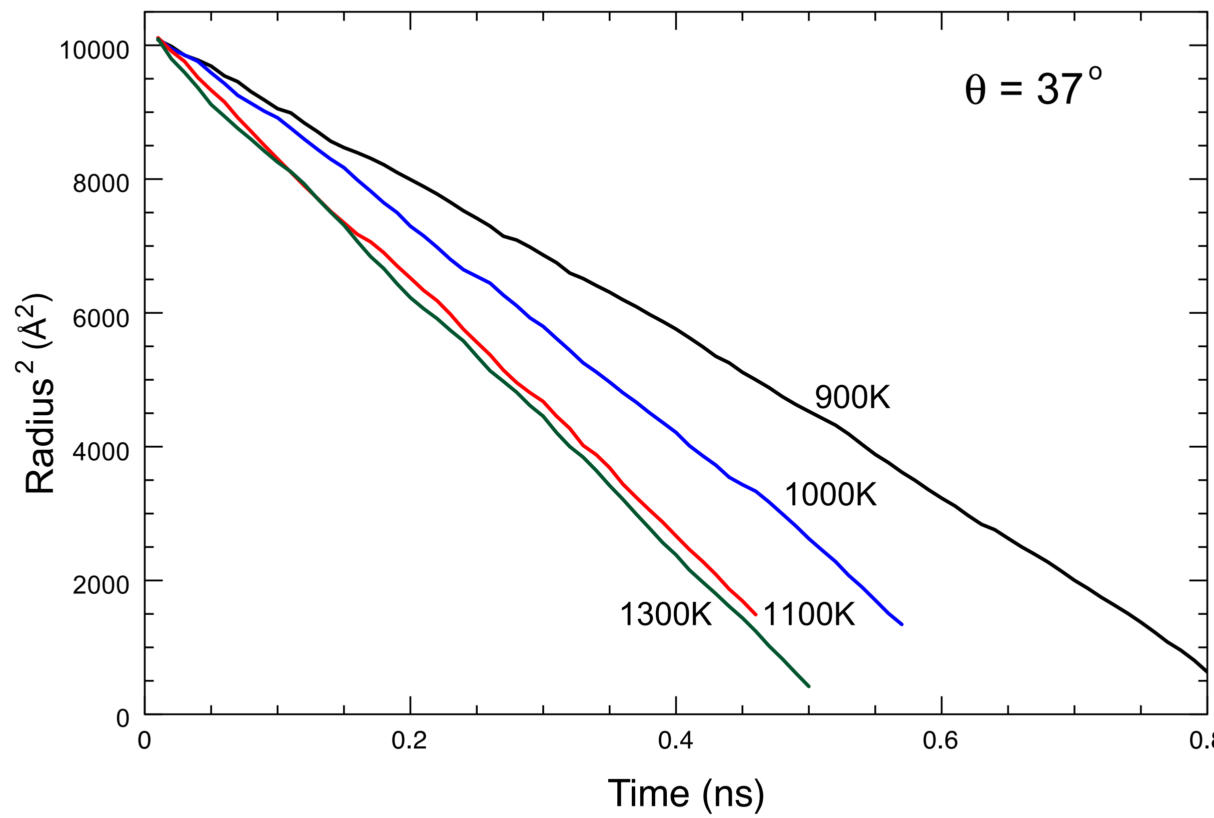
Plots of $R^2 \propto$ time

T = 1300 K ($0.98T_m$)



The coupling disappeared due to high temperature

θ = 37°



Little rotation at all temperatures as if there was no coupling

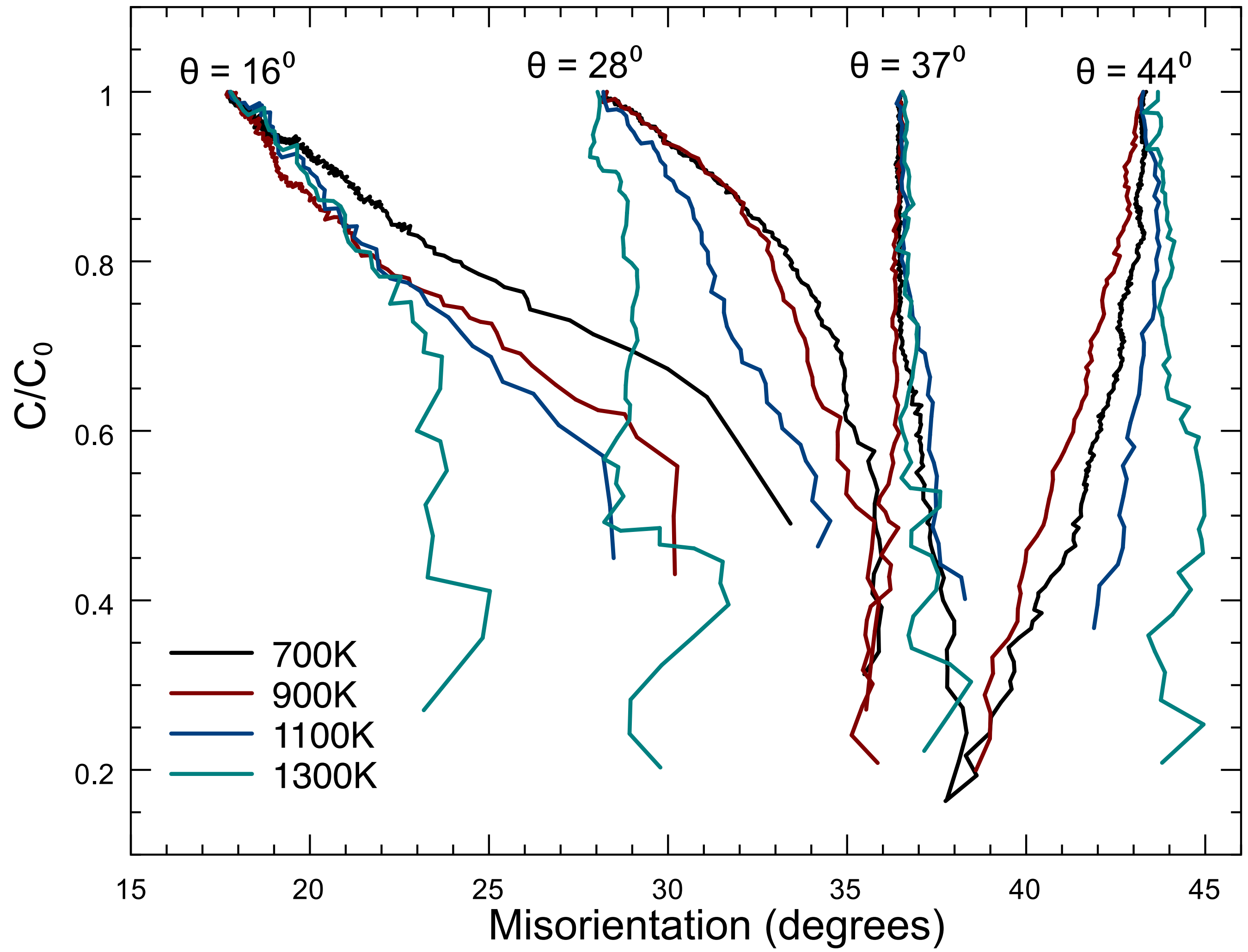
Test of coupling

Limiting case 2: only coupling (no sliding), i.e. V_s=0. The dislocations are conserved.

(Cahn-Taylor, 2004) $$\boxed{-\frac{d\theta}{d\ln R} = \beta(\theta)}$$ This equation can be solved knowing β(θ)

For perfect coupling $\beta(\theta) = 2\tan\frac{\theta}{2}$ → $$\boxed{R\sin\frac{\theta}{2} = const = C}$$

Comparison with simulations



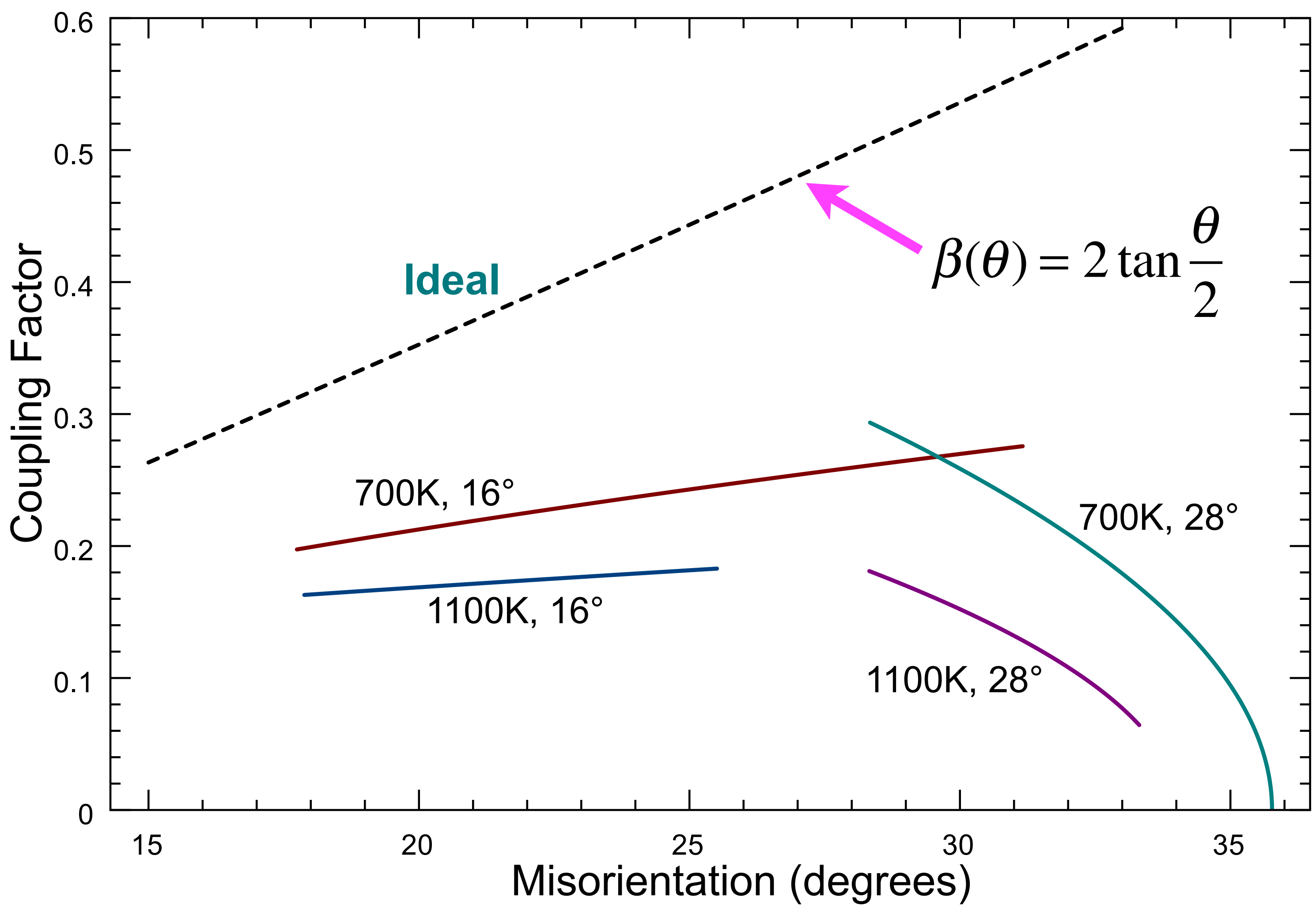
- C is **not** constant at all
- The coupling far from perfect

Test of coupling (continued)

$$\boxed{-\frac{d\theta}{d\ln R} = \beta(\theta)}$$

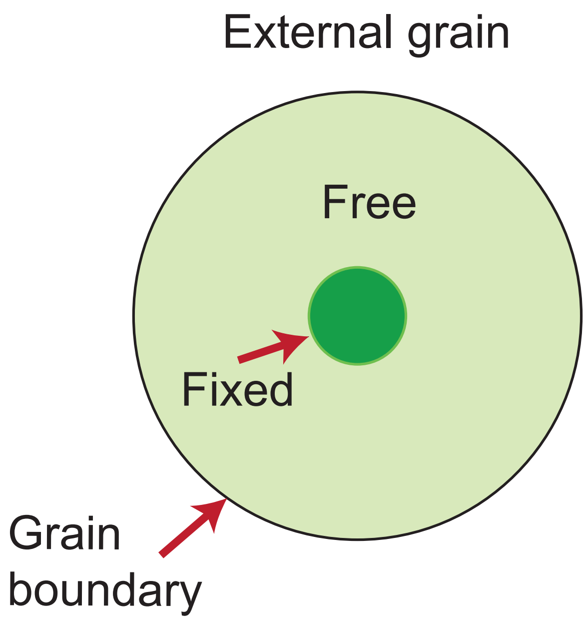
Extract β(θ) from simulations

Comparison with simulations



- The extracted coupling factor is below ideal
- There is less rotation than expected from ideal coupling
- GB sliding is always present

Shrinkage of a fixed grain



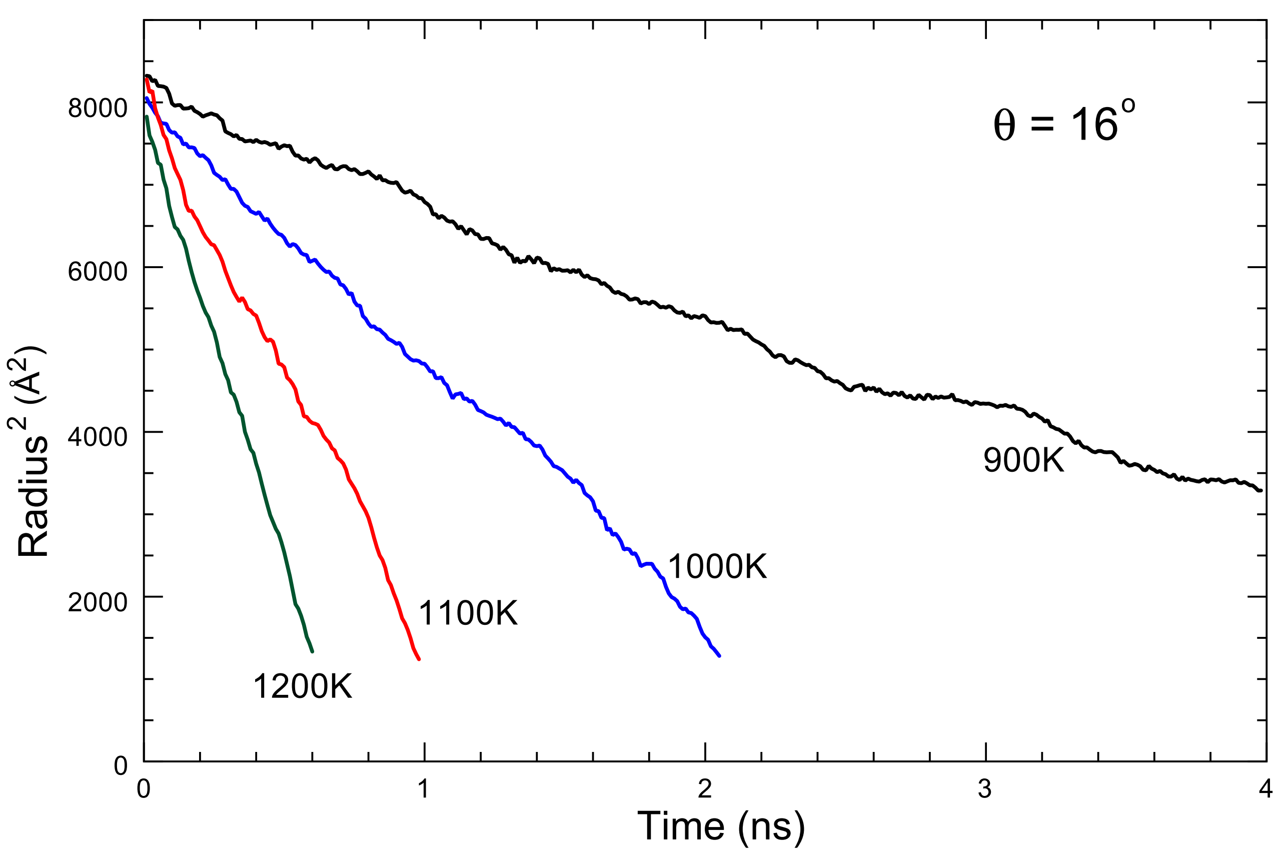
Limiting case 3: No rotation, i.e. $V_{||}=0$

From the Cahn-Taylor equations:

$$V_n = \frac{M_n M_s \gamma}{R\left(\beta^2 M_n + M_s\right)} \rightarrow R^2 = R_0^2 - \frac{2 M_n M_s \gamma}{\left(\beta^2 M_n + M_s\right)} t$$

(Parabolic law)

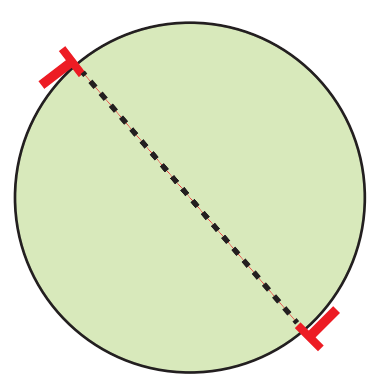
Comparison with simulations



- The fixed core generates back-stresses producing torque on the GB
- The process involves normal GB motion, partial coupling and sliding
- The shrinkage rate is proportional to $M_n M_s$.
- No sliding - no shrinkage
- The dislocation content must decrease!

Two remaining mysteries

- **What happens at θ = 35-37°?**
  - Srinivasan-Cahn: the free-energy cusp at $\Sigma 5$ (θ= 36.9°) is the attractor. Similar ideas: Upmanyu et al. (2006).
  - But the $\Sigma 5$ minimum is very shallow even at T = 0 K.
- **How do the dislocations move without locking each other?**
  - Different dislocations glide on different and intersecting slip planes
  - Srinivasan-Cahn: dislocation annihilation requires glide across the grain, which for large grains is unlikely. Thus the dislocation content must be conserved leading to perfect coupling. But our simulations indicate that the dislocations are not conserved

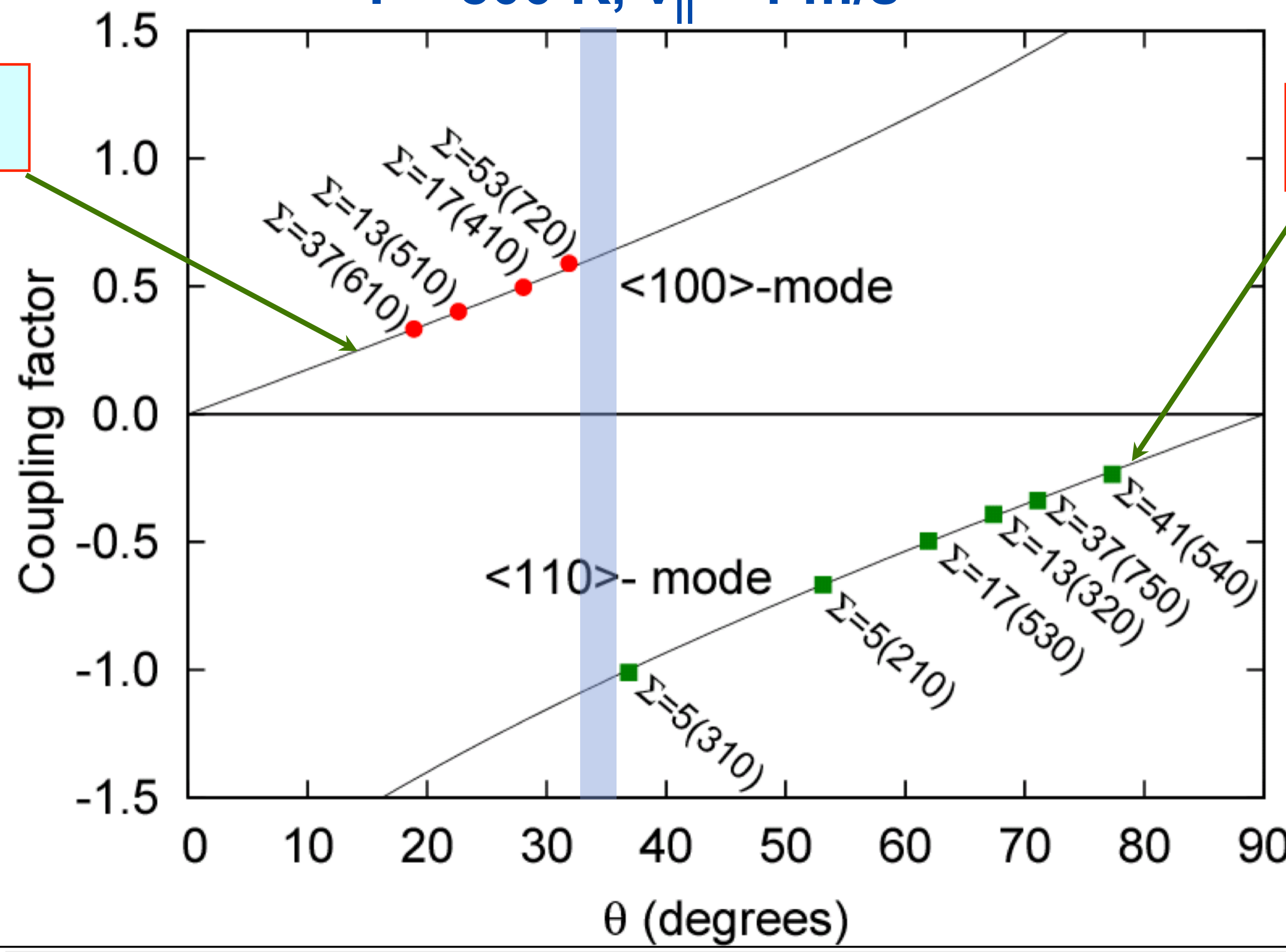


Is this the only way of dislocation annihilation?

Misorientation dependence of β

$T = 800$ K, $v_{||} = 1$ m/s

$\beta = 2\tan(\theta/2)$



$\beta = -2\tan(\pi/4 - \theta/2)$

The points represent MD simulations

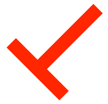
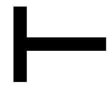
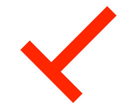
- Excellent agreement between the dislocation model and MD for **all** θ. The Frank-Bilby equation works! The "effective" dislocation content makes sense!
- β is a multivalued geometric factor
- Two modes of coupling: <100>-mode and <110>-mode
- β has a discontinuous change of sign between $\theta=31.9°$ and $\theta=36.9°$

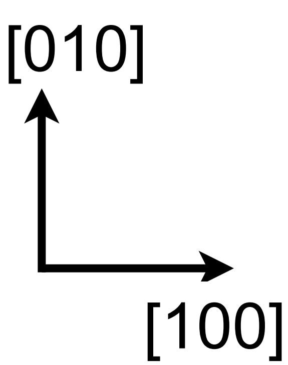
- GBs with θ on the left of the jump have $\beta>0$ and must rotate with increasing θ
- GBs with θ on the right of the jump (e.g. 45^o) have $\beta<0$ and must rotate with decreasing θ
- GBs near the jump will switch between $\beta>0$ and $\beta<0$ with $\langle\beta\rangle \ll 1$ ("frustrated" GBs)

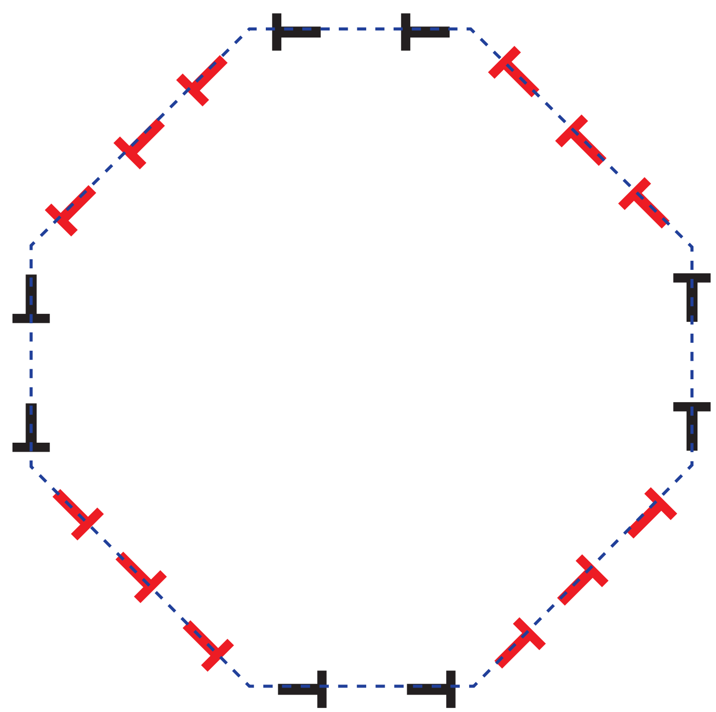
Dislocation models of an enclosed grain

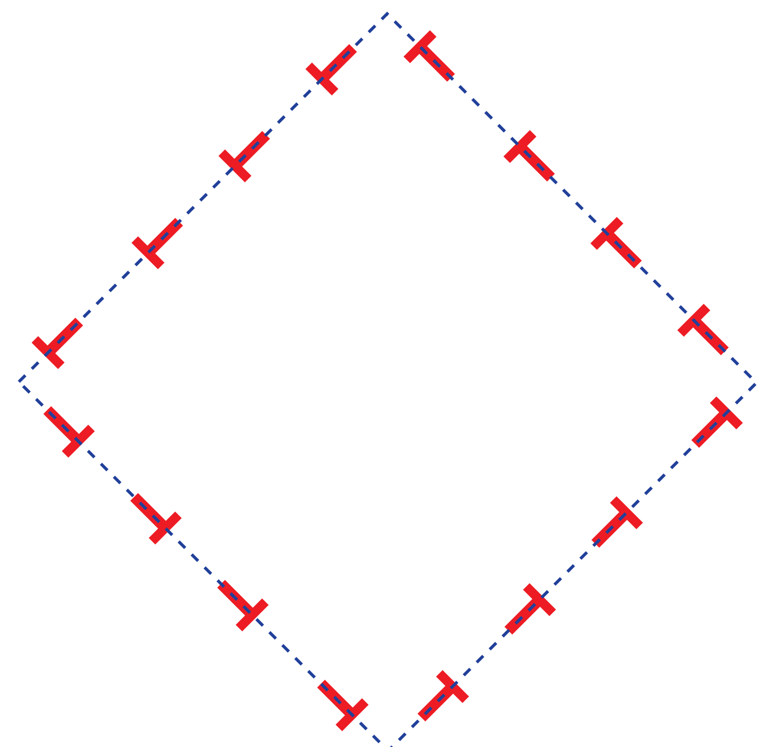
EAM Cu and Al | **Lennard-Jones solid**

Dislocations: 1/2<110> and <100> | 1/2<110>

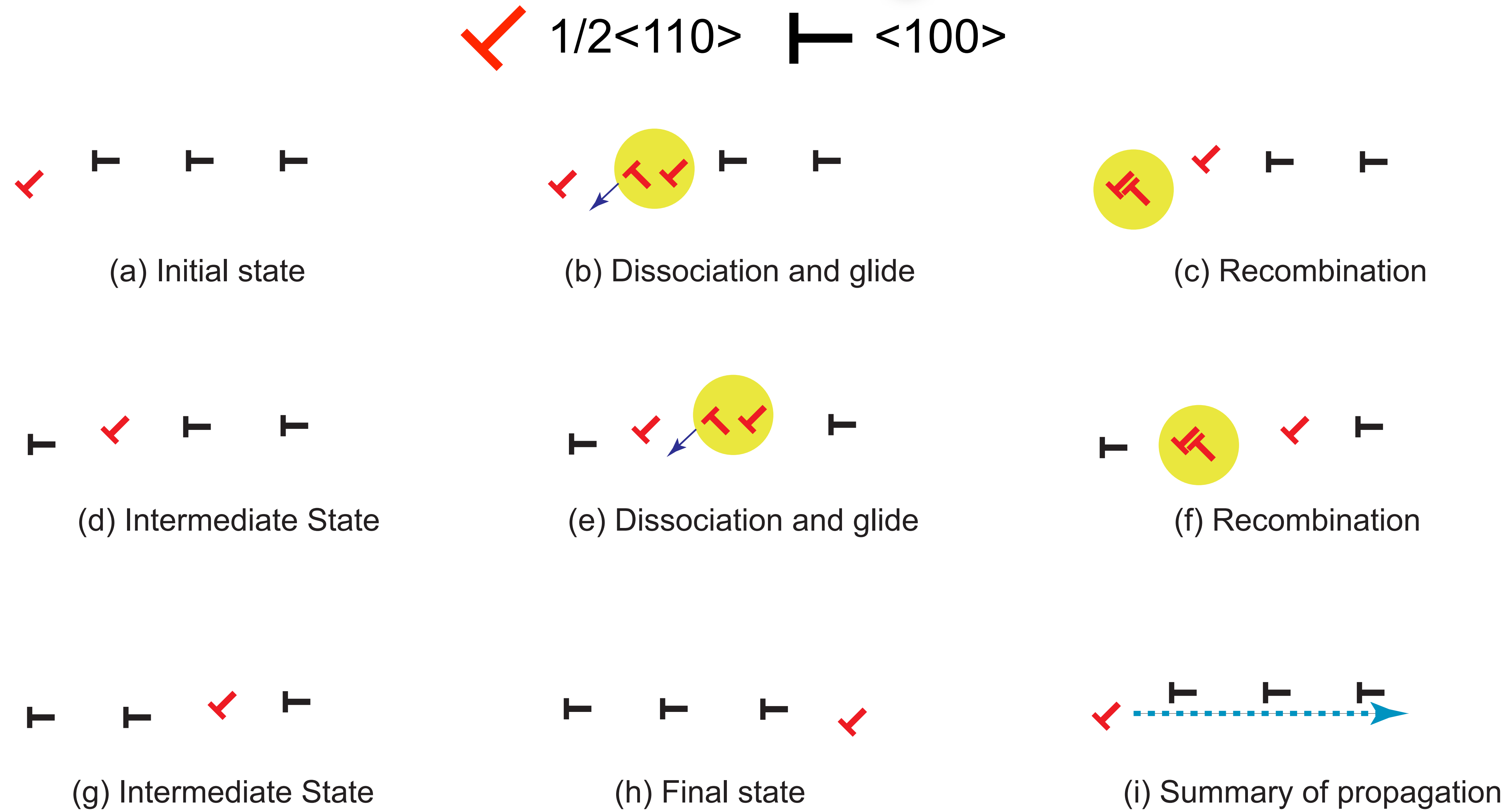




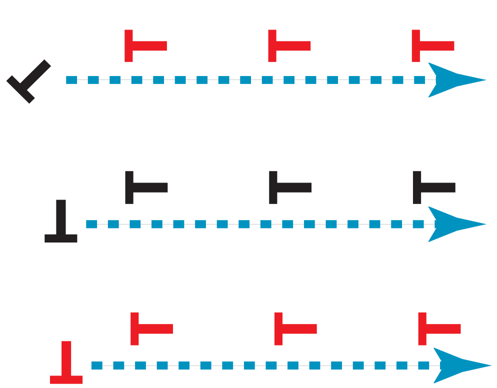


Simulations show that the presence of two types of dislocations enables dislocation reactions leading to dislocation annihilation without crossing the grain.

Dislocation reactions in grain boundaries

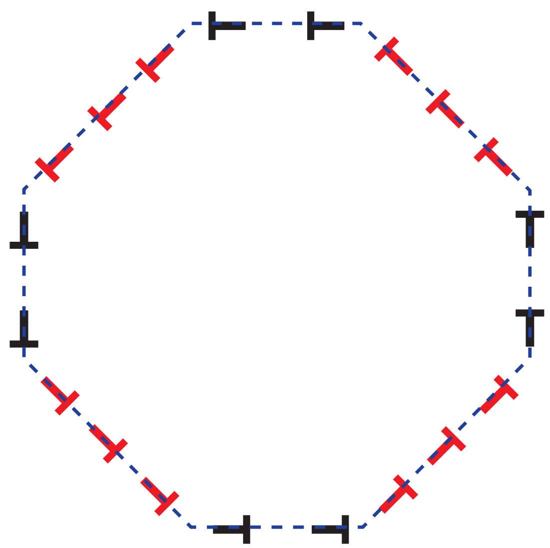


Similar reactions

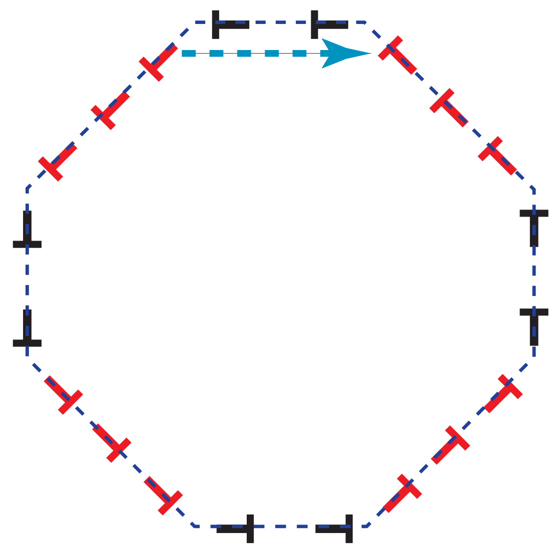


- It is the dislocation content that propagates, not a single dislocation
- This mechanism of motion is different from glide and climb
- There is no annihilation of dislocations

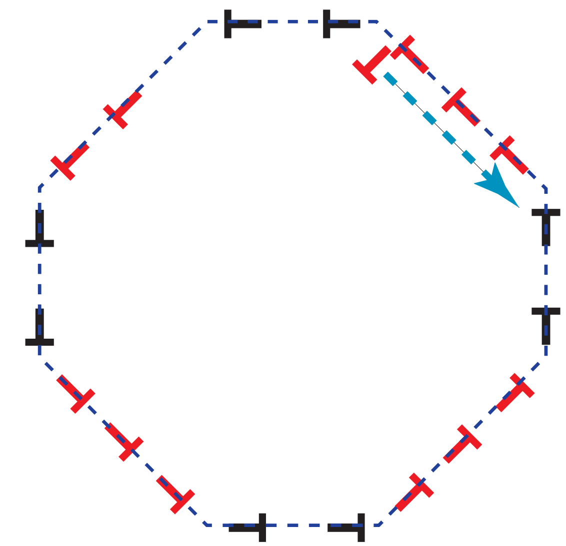
Dislocation annihilation in grain boundaries



(a) Initial state



(b) Propagation



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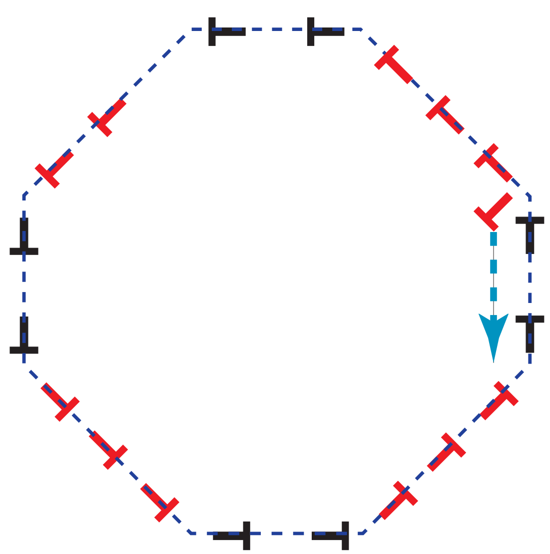
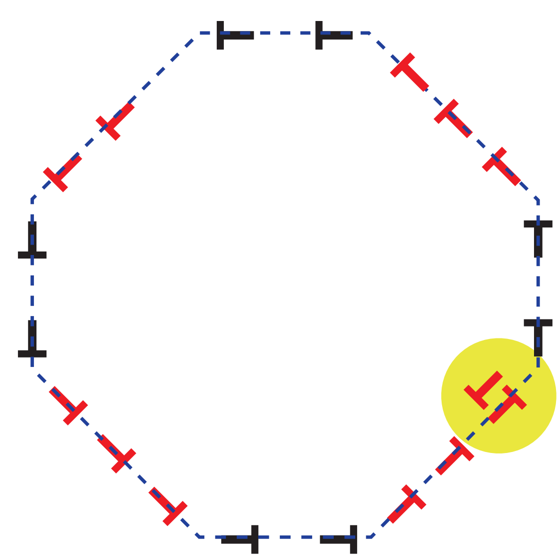
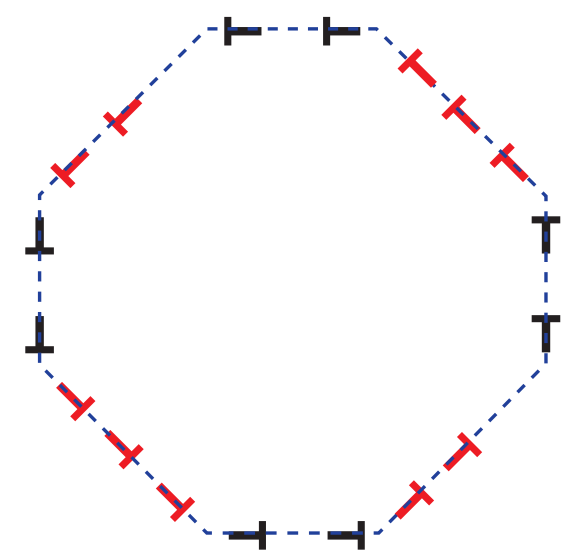


(c) Propagation



(e) Annihilation



(f) Final state

Conclusions

- We applied MD to study capillary driven shrinkage of an isolated cylindrical grain.
- Grain rotation is caused by coupling of GB motion to shear deformation, as proposed by Srinivasan and Cahn (2002).
- The direction of rotation depends on the sign of the coupling factor, which can change with misorientation.
- The rotation stops when the grain reaches a “frustration” angle at which the sign of the coupling factor changes.
- The grain shrinkage is always accompanied by coupling and sliding.
- Sliding of a curved low-angle GB requires a change of its dislocation content, i.e. either annihilation or creation of dislocations.
- In the presence of two types of dislocations, propagation of dislocation content by a chain of dislocation reactions can be responsible for GB motion and dislocation annihilation.
- In the presence of coupling, applied shear stresses can accelerate, retard or even reverse the grain shrinkage, demonstrating stress-induced grain growth.