Energy of low angle grain boundaries based on continuum dislocation structure

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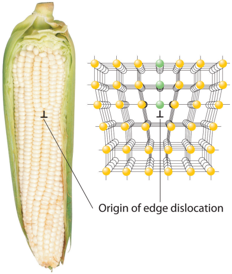
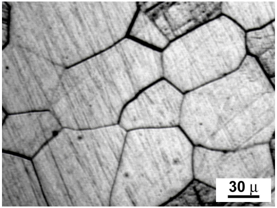
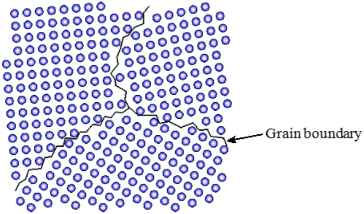
Dislocations and Grain boundaries



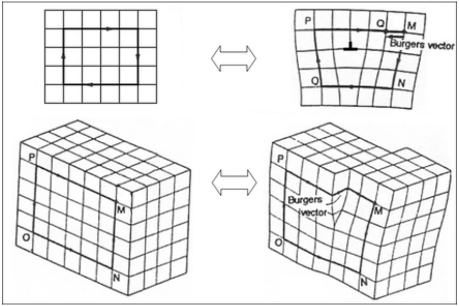
An edge dislocation





Grain Boundaries

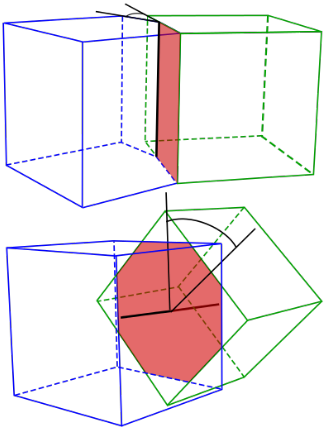
Dislocations: Burgers vectors **b**

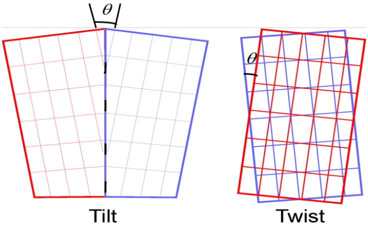


- Edge dislocation: $\mathbf{b} \perp$ dislocation line
- Screw dislocation: $\mathbf{b} \parallel$ dislocation line
- Mixed dislocation: $\mathbf{b}$ has an arbitrary angle with dislocation line

Grain boundaries

- Interface between two single crystals of different orientations



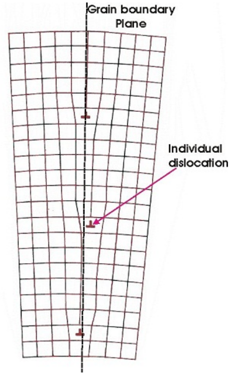


Five degrees of freedom

- Boundary normal vector **n**
- Rotation axis **a**
- Misorientation angle θ

Read-Shockley dislocation model of grain boundaries

W. T. Read, W. Shockley, Phys. Rev. 78 (1950) 275-289.



A low angle tilt grain boundary is modeled by a regular array of dislocations

The unit area energy of grain boundary is

$$E = E_0\theta[A - \ln\theta]$$

where E_0 and A depend on the orientation ϕ of grain boundary.

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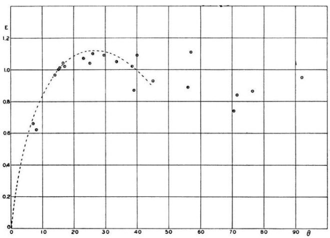
FIG. 2. Energy as a function of θ for grain boundaries. The points show the data of C. G. Dunn for silicon ferrite; see text for orientation. Theoretical curve has $A = 0.231$.



Read-Shockley dislocation model of grain boundaries

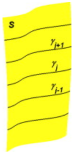
W. T. Read, W. Shockley, Phys. Rev. 78 (1950) 275-289.

- Derived by using **planar** boundaries with **uniform** distributions of **straight** dislocations
- No long-range elastic field (in equilibrium)
- Does not apply to general nonplanar/nonequilibrium grain boundaries
- Does not incorporate global dislocation structure and evolution accurately

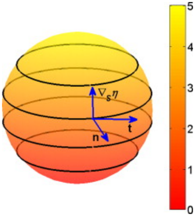
New continuum model

X. Zhu, Y. Xiang, J. Mech. Phys. Solids 69 (2014) 175-194.

- Nonplanar/nonequilibrium low angle grain boundaries
- Enable direct study of global dislocation structure



- Dislocation density potential functions η on S
- The constituent dislocations are given by its contour lines $\eta = j$, for integer j
- Multiple η's for dislocations with multiple Burgers vectors



- the local dislocation line direction $\mathbf{t} = \frac{\nabla_S \eta \times \mathbf{n}}{\|\nabla_S \eta\|}$
- the inter-dislocation distance $D = \frac{1}{\|\nabla_S \eta\|}$
- the surface gradient $\nabla_S \eta = [\nabla - \mathbf{n}(\mathbf{n} \cdot \nabla)]\eta$

The continuum energy

- The elastic energy: $E_S = E_{\text{long}} + E_{\text{local}}$

$$
\begin{aligned}
E_{\text{long}} &= \frac{1}{2}\sum_{i=1}^{J}\sum_{j=1}^{J}\int_S dS_i \int_S dS_j \left[-\frac{\mu}{2\pi}\frac{(\nabla_S \eta_i \times \mathbf{n}_i) \times (\nabla_S \eta_j \times \mathbf{n}_j)\cdot(\mathbf{b}^{(i)} \times \mathbf{b}^{(j)})}{r_{ij}} \right. \\
&\quad + \frac{\mu}{4\pi}\frac{(\nabla_S \eta_i \times \mathbf{n}_i \cdot \mathbf{b}^{(i)}) \times (\nabla_S \eta_j \times \mathbf{n}_j \cdot \mathbf{b}^{(j)})}{r_{ij}} \\
&\quad \left. + \frac{\mu}{4\pi(1-\nu)}(\nabla_S \eta_i \times \mathbf{n}_i \cdot \mathbf{b}^{(i)}) \cdot (\nabla \otimes \nabla r_{ij}) \cdot (\nabla_S \eta_j \times \mathbf{n}_j \cdot \mathbf{b}^{(j)}) \right] \\
E_{\text{local}} &= \sum_{j=1}^{J}\int_S \frac{\mu (b^{(j)})^2}{4\pi(1-\nu)}\left[1 - \nu\frac{(\nabla_S \eta_j \times \mathbf{n}_j \cdot \mathbf{b}^{(j)})^2}{(b^{(j)})^2 \|\nabla_S \eta_j\|^2}\right] \|\nabla_S \eta_j\| \log\frac{1}{r_g \|\nabla_S \eta_j\|} dS_j
\end{aligned}
$$

Grain boundaries at equilibrium state

At equilibrium state,

- the long range elastic field cancels out
- a grain boundary with rotation angle θ, rotation axis $\mathbf{a}$ satisfies Frank's formula

$$\mathbf{B}(\mathbf{V}) = \theta(\mathbf{V} \times \mathbf{a}) = \sum_j \mathbf{b}^{(j)}(\nabla_S \eta_j \cdot \mathbf{V}), \qquad \text{any } \mathbf{V} \text{ in gain boundary}$$

- Frank's formula cannot determine a unique solution.

Grain boundaries at equilibrium state

- Constrained Minimization Problem (CMP)

$$\text{minimize} \quad E = \int_S \gamma_{gb} dS,$$

$$\text{with} \quad \gamma_{gb} = \sum_{j=1}^{J} \frac{\mu (b^{(j)})^2}{4\pi(1-\nu)} \left[1 - \nu \frac{(\nabla \eta_j \times \mathbf{n}_j \cdot \mathbf{b}^{(j)})^2}{(b^{(j)})^2 \|\nabla \eta_j\|^2} \right] \|\nabla \eta_j\| \log \frac{1}{r_g \sqrt{\|\nabla \eta_j\|^2 + \epsilon}},$$

$$\text{subject to} \quad \mathbf{h} = \theta(\mathbf{V} \times \mathbf{a}) - \sum_j \mathbf{b}^{(j)} (\nabla \eta_j \cdot \mathbf{V}) = 0.$$

Numerically the CMP can be solved by penalty method

- Unconstrained Minimization Problem (UMP)

$$\text{minimize} \ Q = \int_S \left(\gamma_{gb} + \frac{1}{2} \alpha ||h||^2 \right) dS,$$

  where $\alpha > 0$ with large value is the penalty parameter.
- UMP converges to CMP as $\alpha \to \infty$.

Planar grain boundary

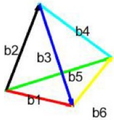
- This unconstrained minimization problem (UMP) is still challenging due to the nonconvexity of the boundary energy.
- Considering uniform distribution of straight dislocations, $\nabla \eta_j = (\eta_{jx}, \eta_{jy})$.
- UMP can be solved by the gradient minimization method.
- The evolution equations are

$$
\begin{aligned}
(\eta_{jx})_t &= -\left(\frac{\partial \gamma_{gb}}{\partial \eta_{jx}} + \alpha \frac{\partial p}{\partial \eta_{jx}}\right), \\
(\eta_{jy})_t &= -\left(\frac{\partial \gamma_{gb}}{\partial \eta_{jy}} + \alpha \frac{\partial p}{\partial \eta_{jy}}\right),
\end{aligned}
$$

where $p = ||h||^2/2$.

Simulation

- Apply this model to Face Centered Cubic (FCC)
- Set directions $[1,1,1],[\bar{1},1,0],[\bar{1},\bar{1},2]$ as the x,y,z directions
- Six Burger's vectors

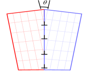


$$\mathbf{b}^{(1)}=(0,b,0),\mathbf{b}^{(2)}=(0,\frac{b}{2},\frac{\sqrt{3}}{2}b),\mathbf{b}^{(3)}=(0,\frac{b}{2},-\frac{\sqrt{3}}{2}b),$$

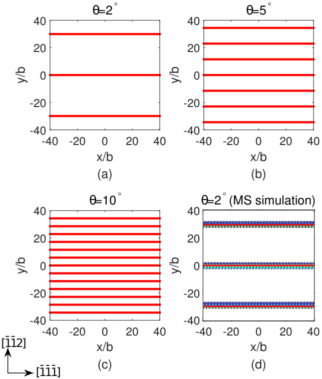
$$\mathbf{b}^{(4)}=(\frac{\sqrt{6}}{3}b,0,\frac{\sqrt{3}}{3}b),\mathbf{b}^{(5)}=(-\frac{\sqrt{6}}{3}b,\frac{b}{2},\frac{\sqrt{3}}{6}b),\mathbf{b}^{(6)}=(-\frac{\sqrt{6}}{3}b,-\frac{b}{2},\frac{\sqrt{3}}{6}b),$$

where b is the length of Burgers vectors.

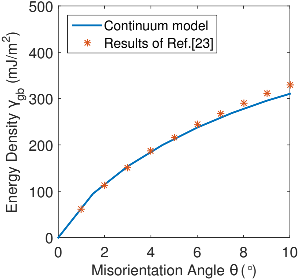
[110]tilt grain boundary (different misorientation θ)



Dislocation structure: $\theta = \frac{\pi}{60}, \frac{\pi}{36}, \frac{\pi}{18}, \frac{\pi}{9}$



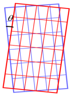
Energy comparison with MD simulation (Al, EAM potential)



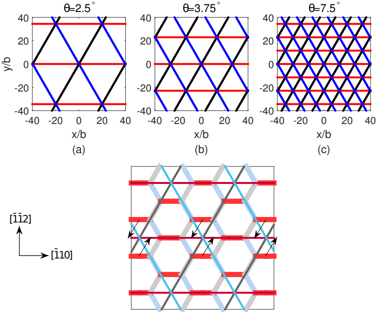
Dislocation density

θ	$\pi/60$	$\pi/36$	$\pi/18$	$\pi/9$
Analytical Value (1/b)	0.0524	0.0873	0.1745	0.3491
Continuum Model (1/b)	0.0522	0.0872	0.1745	0.3490

[111]twist grain boundary (different misorientation θ)



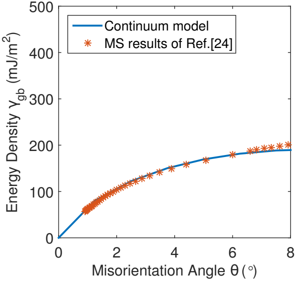
Dislocation structure: $\theta = \frac{\pi}{72}, \frac{\pi}{48}, \frac{\pi}{36}, \frac{\pi}{24}$



(a) (b) (c)

(d)

Energy comparison with MD simulation (Al, EAM potential)

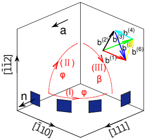


Dislocation density

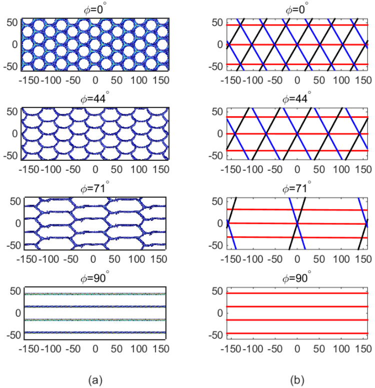
θ	$\pi/72$	$\pi/48$	$\pi/36$	$\pi/24$
MD Simulation (1/b)	0.0282	0.0424	0.0565	0.0847
Continuum Model (1/b)	0.0291	0.0436	0.0582	0.0873

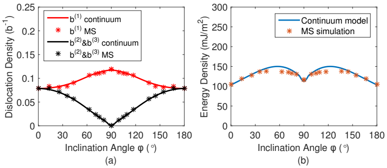
Fixed

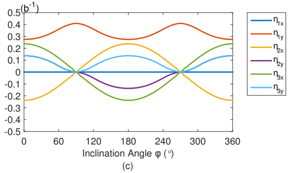
- rotation axis [111]
- misorientation $\theta = 1.95^\circ$



Dislocation structure comparison with MD simulation

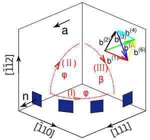


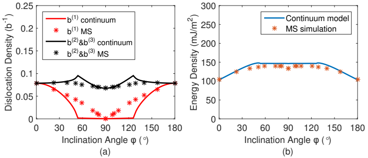


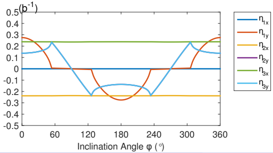


Fixed

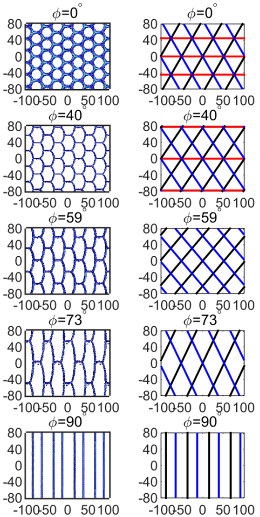
- rotation axis [111]
- misorientation $\theta = 1.95^\circ$







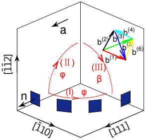
Dislocation structure comparison with MD simulation

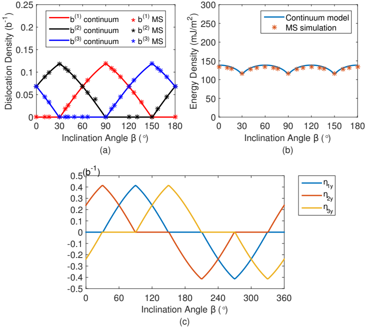


GBs with different orientations: (III) rotating around [111]

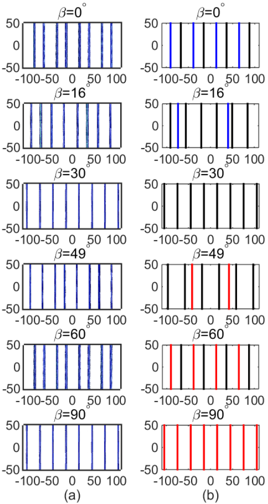
Fixed

- rotation axis [111]
- misorientation $\theta = 1.95^\circ$





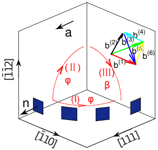
Dislocation structure comparison with MD simulation



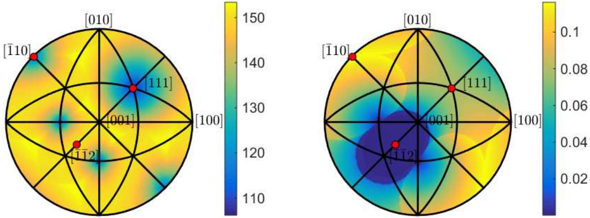
GBs with any orientation

Fixed

- rotation axis [111]
- misorientation $\theta = 1.95^\circ$



Grain boundary energy (a) and dislocation density (b) in stereography projection

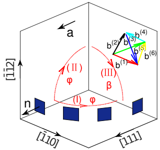


(a) (b)

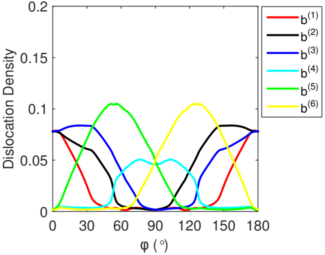
GBs as rotation axis varies

Fixed

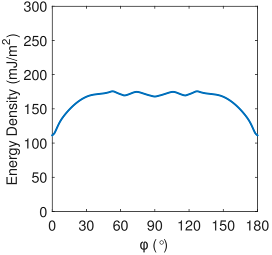
- boundary plane $n = (111)$
- misorientation $\theta = 1.95^\circ$



Dislocation density (a) and grain boundary energy density (b) as **a** varying along path (I)



(a)



(b)

Summary and On-going work

Summary

- Continuum model for dislocation structure and energy of low angle GBs (nonplanar, nonequilibrium)
- Numerical method for structure and energy of low angle planar GBs (arbitrary boundary, rotation axis)
- Numerical simulation for structure and energy in fcc

On-going work

- Nonplanar grain boundary
- Dynamic problem: grain boundaries are not fixed
- Nonequilibrium state: long-range energy E_{long}

Thank you!