A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and in-coming dislocations

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What is a dislocation?

Dislocations are perturbations of the perfect crystal along a line. A dislocation is characterized by its line sense (l) and Burgers vector (b).
Dislocations develop during

1) crystallization from melt
e.g. semiconductor thin film

2) plastic deformation
e.g. Ni-based superalloys

Why people study dislocations?

Dislocation motion, multiplication, and self-organization determine many physical and mechanical material properties, e.g. electrical resistivity of semiconductors, strength and fatigue failure of metals.

Bending of a metal paper clip:
1) irreversible (plastic) deformation
2) strain hardening

Formability (metal forming)
Strength (under working condition)
Study dislocations with dislocation dynamics models

- Stress field of a straight dislocation segment

\[
\sigma_{ij}(P) = \frac{\mu}{8\pi} \int_{L} R_{mnp} b_n (\varepsilon_{jmn} dL_i + \varepsilon_{imn} dL_j) \\
+ \frac{\mu}{4\pi(1-\nu)} \int_{L} b_n \varepsilon_{kmn} (R_{ijm} - \delta_{ij} R_{mpn}) dL_k,
\]

- \( R = P - Q \) is the vector connecting the point of interest \( P \) and a source point \( Q \) on the dislocation segment \( L \),
- \( R_{ijk} \equiv \frac{\partial^3 R}{\partial L_i \partial L_j \partial L_k} \), \( \varepsilon_{ijk} \) is the permutation symbol, and \( \delta_{ij} \) is the Kronecker delta.

- Peach-Koehler equation

\[
f_{\text{node}} = (\sigma_{\text{net}} + \sigma_{\text{ext}}) \cdot b \times t
\]

- Mobility function

\[
v_{\text{node}} = M (f_{\text{node}})
\]
The dislocation dynamics (DD) model

ParaDiS code (http://paradis.stanford.edu)
[Arsenlis A. et al., 2007, MSMSE]
- singularity of classical elasticity theory
  - based on a non-singular continuum theory
    [Cai W. et al., 2006; JMPS]
- high computational cost of long-range stress evaluation, $N^2 \rightarrow N$
  - developed the multipolar representation of long-range stress field
- parallel computing, $N/n_{cpu}$
  - dynamic domain decomposition
- topology update
  - Mergenode & Splitnode
courtesy of LLNL ParaDiS team
dislocation dynamics model development

- dislocation–low angle grain boundary interactions  
  - model modifications that enable the ParaDiS code to run simulations in laboratory frames
  - implement the mobility law for binary junctions
- high temperature creep in nickel-based single crystal superalloys  
  [Liu B., Raabe D., Roters F., Multiscale Materials Modeling (MMM) conference 2012, Singapore]
  - model modifications that enable dislocation climb driven by mechanical and chemical forces
  - calculation of biaxial misfit stresses in the matrix channels
  - implementation of antiphase boundary back force in the precipitates
Research using DD simulations at MPIE

- **LAGB**
- **bending**
- **nanoindentation**
- **glide**
- **glide + climb**

Interfacial dislocation network in superalloys
Strengthening ability of low angle grain boundaries?

Some coherent boundaries (such as low angle GBs) are not effective at resisting lattice dislocation penetration.

Lu K., Lu L. and Suresh S., 2009, Science
A single set of edge dislocations

A symmetrical tilt low angle grain boundary
Hexagonal dislocation network

A general low angle grain boundary of mixed character
Method and feasibility

Lomer-Cottrell lock, MD

Lomer-Cottrell lock, TEM

Lomer-Cottrell lock, MD

Lomer-Cottrell lock, DD

Collinear annihilation, MD-DD
Madec R. et al., 2003, Science

ternary junction, MD-TEM
Bulatov V.V. et al., 2006, Nature

ternary junction, DD
Determination of penetration resistance

Determination of penetration resistance

Liu B., Eisenlohr P., Roters F., Raabe D.,
2012, Acta Mater., In press
Implications

- The strength of low angle grain boundaries (LAGBs) against dislocation penetration has been studied with dislocation dynamics (DD) simulations. The transmission resistance is found to be dependent on the slip system and line sense of the incident dislocation, which is directly related to the short-range dislocation interactions between the incident and LAGB dislocations.

- When one slip system is activated, the positive and negative dislocations intersect the LAGB from opposite sides of the LAGB plane. If the transmission resistance difference is significant between the anti-parallel incident dislocations, asymmetrical transmission phenomena or even one side penetration can occur. When multiple slip systems are activated, the LAGB allows free dislocations on some of the slip systems to pass by more easily than on others due to the different dislocation interaction strengths with the LAGB dislocations.
Influence of low angle grain boundary on free dislocation multiplication and dislocation structure evolution (ongoing)

Frank-Read sources alone

LAGB + Frank-Read sources
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Total DDV $(\rho^+ - \rho^-)$ profile along the normal of the LAGB for active slip systems
Influence of low angle grain boundary on free dislocation multiplication and dislocation structure evolution (ongoing)

Geometrically necessary DDV \( (\rho^+ + \rho^-) \) profile along the normal of the LAGB for active slip systems
Influence of low angle grain boundary on free dislocation multiplication and dislocation structure evolution (ongoing)

Remarks

Low angle grain boundary
(1) regulates dislocation multiplication on different slip systems
(2) and separates dislocation content on the same slip system, which can be explained by
the polarization of LAGB penetration resistance among slip systems and incident dislocations of opposite signs.

The simulation results have implications on dislocation microstructure evolution during plastic deformation concerning
(1) disorientation increase of low angle grain boundary,
(2) formation of geometrically necessary boundary,
(3) and grain subdivision.
Dislocation pattern, density, internal stress (ongoing)
Jakobsen B. et al., 2006, Science
Dislocation pattern, density, internal stress (ongoing)
Dislocation pattern, density, **internal stress** (ongoing)
Experimental determination of dislocation pattern, density and internal stress is not an easy task.
0.1%  0.3%  0.5%  1%  2%  3%
PRA025

Density (m⁻²)

2.5e15
1.25e15
1e12
Dislocation pattern, density, internal stress (ongoing)

Remarks

(1) mutual validation of dislocation dynamics models and experimental techniques (TEM, ECCI, X-ray diffraction)

(2) observation and understanding of the evolution of dislocation pattern, density field and internal stress field at early deformation stage

(3) extraction of dislocation density and stress correlation functions for the development of statistical dislocation models
Future polycrystal simulations need a coarse-grained model for high angle grain boundary.

This work (PRA025) studied single crystal and bicrystals separated by low angle grain boundary.