Dislocation Dynamics
for Computational Design of Thin Film Systems

Lizhi Sun
Department of Civil and Environmental Engineering
and Center for Computer-Aided Design
The University of Iowa

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Large-scale Dislocation Dynamics Simulations for Computational Design of Thin Film Systems

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PIs: N.M. Ghoniem (UCLA)  Lizhi Sun (Univ. of Iowa)
Post-doc: X.L. Han (UCLA)  Students: E.H. Tan (U. Iowa)
                                 H.T. Liu (U. Iowa)
                                 Z.Q. Wang (UCLA)
Materials Modeling in Terms of Length Scales

- *Ab initio* method
- Molecular dynamics method
- Dislocation dynamics method
- Finite element method
Project Objectives

• Investigating single and collective dislocation activities in anisotropic materials, which determines the mechanical behavior of semiconductor thin film systems.

• Coupling dislocation dynamics with continuum mechanics to consider the surface and interface effects.
Project Objectives (Cont’d)

• Applying dislocation dynamics software to investigate a number of physical mechanisms including misfit and threading dislocation motion, annihilation, multiplication, interaction, and junction; dislocation interaction with point defects, precipitates and inclusions; thermal residual stress effect; design of buffer layers and superlattices, etc.

• Conducting large-scale simulation and optimization of semiconductor systems to provide guidelines for engineering design of microelectronics.
Presentation Outline

1. Anisotropic Dislocation Dynamics Approach

2. Dislocation Interaction with Inclusions

3. Dislocations in Thin Films
Elastic Fields of Dislocation Loops in Anisotropic Materials

Mura formula:

\[ \sigma_{ij}(x) = C_{ijkl} \beta_k(x) \]

\[ \beta_j(x) = \frac{1}{8\pi^2} \epsilon_{ijk} b_i \frac{d}{dl} \left( \frac{r}{L} \right) I_{ik}(m,n) dl \]

\[ I_{ik}(m,n) = \frac{2\pi}{m} \left\{ \frac{m_i N_{ik} (-m \sin \phi + n \cos \phi)}{D(-m \sin \phi + n \cos \phi)} - \cos \phi \frac{n_i N_{ik} (-m \sin \phi + n \cos \phi)}{D(-m \sin \phi + n \cos \phi)} - \frac{N_{ik}(n)}{D(n)} \right\} d\phi \]
Dislocation Dynamics in Anisotropic Materials

- Equation of Dislocation Motion (variational weak form)

\[ \int_{\Gamma} \left( f_i^t - B_{ij} V_j \right) \delta r_i \left| ds \right| = 0 \]

- \( f \): Forces (external, internal, self force, and friction resistant (Perierls) force, etc.)
- \( B \): Resistive matrix (inverse mobility)
- \( V \): Dislocation movement
Dislocation Dynamics in Anisotropic Materials

**Self-force (Barnett)**

\[ F = \kappa E(t) - \kappa [E(t) + E''(t)] \ln[8/\varepsilon\kappa] - J(L, P) + F_{\text{core}} \]

- **Stretch**
- **Line Tension**
- **Non-local**

\[ F = \kappa E(t) - 0.5[\sigma_{ij}(P_1) + \sigma_{ij}(P_2)]b_in_j \]
Circular dislocation loop on the plane (1,1,1)

Slip direction [-1,1,0]  Loop radius R
Dislocation Dynamics in Anisotropic Materials

Anisotropic Ratio
\[ A = \frac{2C_{44}}{(C_{11} - C_{12})} \]

Stress \( \sigma \) (divided by \( 0.5(C_{11} - C_{12})b/R \))
Dislocation Dynamics in Anisotropic Materials

Isotropic $A=1$

Anisotropic $A=0.5$
Dislocation Dynamics in Anisotropic Materials

\[ \mathbf{b} = \frac{1}{2} [\overline{1} 0 1] \]

Parallel plane (111) separated

\[ h = 25\sqrt{3}a \]

No applied load
Dislocation Dynamics in Anisotropic Materials

\[ \frac{1}{2} [01 \bar{1}] (11\bar{1}) \text{ and } \frac{1}{2} [101] (11\bar{1}) \]
Dislocation Interaction with Inclusions
Dislocation Loops Interacting with Heterogeneous Inclusions

\[ \varepsilon^*_i = -[S_{ijkl} + (C^*_{i m n} - C^*_{i m n})^{-1}C_{m n l}]^{-1}\varepsilon^d_{ij} \]
Dislocation Loops Interacting with Heterogeneous Inclusions

\[ \sigma_{ij}(x) = \sigma_{ij}^{df}(x) + \sigma_{ij}^{\prime}(x) \]

\[ \sigma_{ij}^{\prime}(x) = C_{ijkl} \bar{\sigma}_{klmm}(x) \varepsilon_{mn}^{*} \]
Dislocation Loops Interacting with Heterogeneous Inclusions

\[ \sigma_{ij}(x) = \sigma_{ij}^{d-total}(x) + \sum_{m} \sigma'_{ij}(x)\sigma_{ij}^{d-total}(x) \]

\[ \sigma_{ij}^{d-total}(x) = \sum_{n} \sigma_{ij}^{d_n}(x) \]
Dislocation Loops Interacting with Heterogeneous Inclusions

Dislocation Loop: \( R = 100 \, b \)

Particle: \( r = 20 \, b \)

Particle center: \((R, 0, 0.4R)\)

Constants of Materials: \( E_m = 73 \, \text{GPa}, \nu_m = 0.33 \)

\( E_p = 485 \, \text{GPa}, \nu_p = 0.20 \)
Dislocation Loops Interacting with Heterogeneous Inclusions

\[ \sigma_{xx} \text{ (GPa)} \]

\[ \sigma_{xz} \text{ (GPa)} \]

Without Particle

With Particle
Dislocation Loops Interacting with Heterogeneous Inclusions

\begin{align*}
\sigma_{yy} \text{ (GPa)} & \quad \text{Without Particle} \quad \text{With Particle} \\
\sigma_{zz} \text{ (GPa)} & \quad \text{Without Particle} \quad \text{With Particle}
\end{align*}

\begin{align*}
\text{Without Particle} & \quad z/R \\
\text{With Particle} & \quad z/R
\end{align*}
Dislocations in Thin Films
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

\[
\sigma_{ij}(x) = C_{ijkl}u_{k,l}(x)
\]

\[
u_m(x) = -\int_{AV} b_{i} n_{j} C_{ijkl}^{I} \frac{\partial}{\partial x_l} G_{km}(x', x) dA
\]

\[
G_{km}(x', x) = ?
\]
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

\[ C_{ijkl}^{I} = \frac{1}{G_{km}(x', x)} + \sigma_{ij} n_j \]

Rongved Solution

Integral Transforms
Elastic Fields of Dislocation Loops in the Film-Substrate Systems
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

- $E_\text{f}=85.5\text{GPa}$, $v_\text{f}=0.31$, $E_\text{s}=165.5\text{GPa}$, $v_\text{s}=0.25$
- $h_\text{f}=0.1\mu\text{m}$, $R=0.25\mu\text{m}$, $x_1=0.0$, $x_2=0.05\mu\text{m}$

Graph showing stress distribution for different domains:
- Half-space
- Film-substrate
- Infinite domain
- Two half-space

$L.\ Sun$

The University of Iowa
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

\[ E_f = 85.5 \text{GPa}, \nu_f = 0.31, E_s = 165.5 \text{GPa}, \nu_s = 0.25 \]
\[ h_f = 0.1 \mu m, R = 0.25 \mu m, x_1 = 0.0, x_2 = 0.05 \mu m \]

\[ \sigma_{32}h/b(\text{GPa}) \]

- Half-space
- Infinite domain
- Film-substrate
- Two half-space
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

\[ E_f = 85.5 \text{GPa}, \nu_f = 0.31, E_s = 165.5 \text{GPa}, \nu_s = 0.25 \]
\[ h_f = 0.1 \mu m, R = 0.25 \mu m, x_1 = 0.0, x_2 = 0.05 \mu m \]
Summary

- Dislocation activities in anisotropic materials (UCLA Team)

- Dislocation interaction with inclusions and precipitates (Univ. of Iowa Team)

- Dislocation statics in thin film – substrate systems (Univ. of Iowa Team)