Dislocation Dynamics
for Computational Design of Thin Film Systems

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Collaborative ITR/AP Research on

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

(September 2001 – August 2004)

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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.

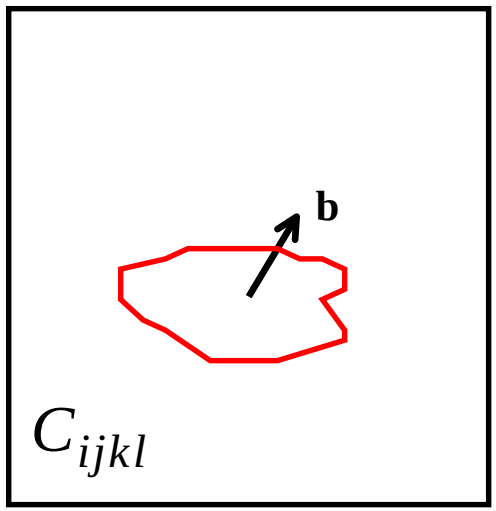
Presentation Outline

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:

$$\sigma_{ij}(\boldsymbol{x}) = C_{ijkl}\beta_{lk}(\boldsymbol{x})$$

$$\beta_{ji}(\boldsymbol{x}) = \frac{1}{8\pi^2} \in_{jnh} C_{klmn} b_m \oint_L \frac{d}{dl}\left(\frac{\nu_h}{r}\right) I_{lik}(\boldsymbol{m},\boldsymbol{n}) dl$$

$$I_{lik}(\boldsymbol{m},\boldsymbol{n}) = \int_0^{2\pi} \left\{ \frac{m_l N_{ik}(-\boldsymbol{m}\sin\phi + \boldsymbol{n}\cos\phi)}{D(-\boldsymbol{m}\sin\phi + \boldsymbol{n}\cos\phi)} - \frac{\cos\phi}{\sin\phi} n_l \left[\frac{N_{ik}(-\boldsymbol{m}\sin\phi + \boldsymbol{n}\cos\phi)}{D(-\boldsymbol{m}\sin\phi + \boldsymbol{n}\cos\phi)} - \frac{N_{ik}(\boldsymbol{n})}{D(\boldsymbol{n})} \right] \right\} d\phi$$

Dislocation Dynamics in Anisotropic Materials

- **Equation of Dislocation Motion (variational waek form)**

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

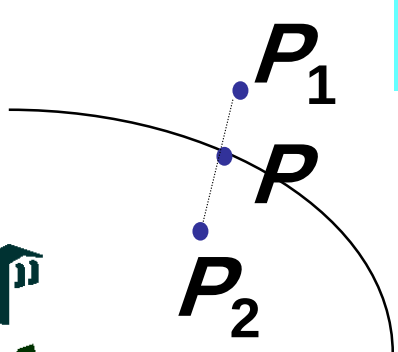
- ***f*: Forces (external, internal , self force, and friction resistant (Perierls) force, etc.)**
- ***B*: Resistive matrix (inverse mobility)**
- ***V*: Dislocation movement**

Dislocation Dynamics in Anisotropic Materials

- **Self-force (Barnett)**

$$F = \underbrace{\kappa E(t)}_{\text{Stretch}} - \underbrace{\kappa[E(t) + E''(t)]\ln[8/\varepsilon\kappa)]}_{\text{Line Tension}} - \underbrace{J(L,P)}_{\text{Non-local}} + F_{core}$$

$$F = \kappa E(t) - 0.5[\sigma_{ij}(P_1) + \sigma_{ij}(P_2)]b_i n_j$$

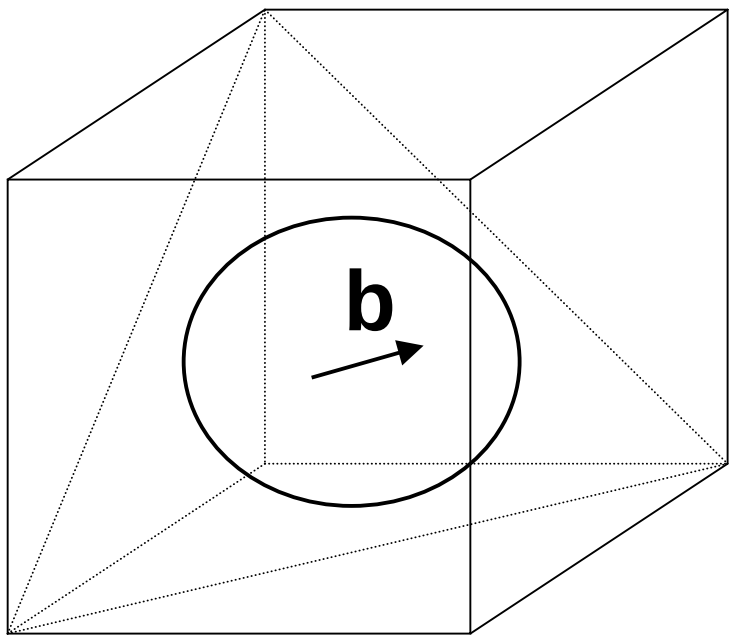


Dislocation Dynamics in Anisotropic Materials

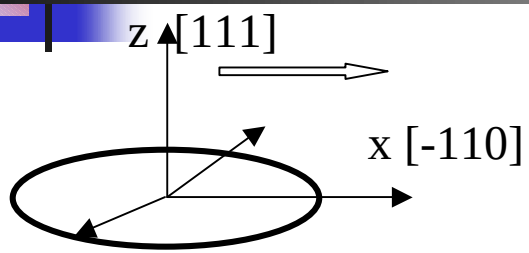
Circular dislocation loop on the plane (1,1,1)

Slip direction [-1,1,0]

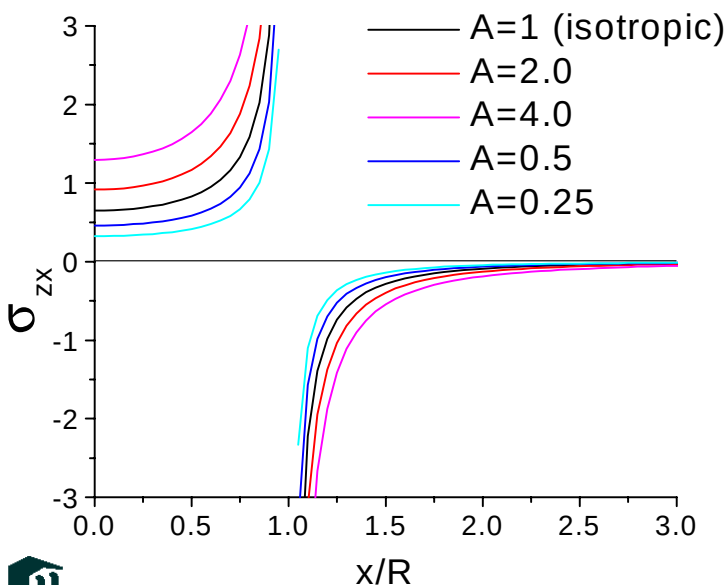
Loop radius R

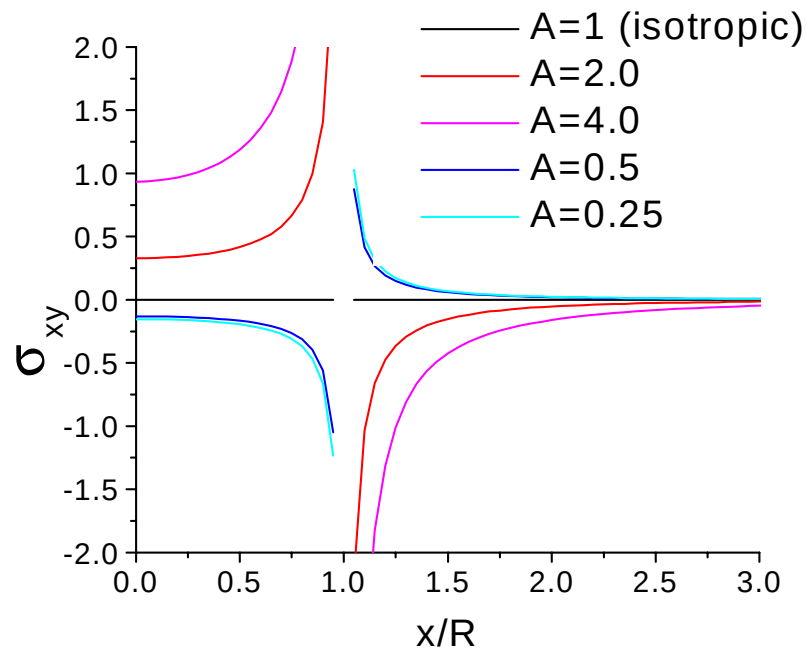


Dislocation Dynamics in Anisotropic Materials



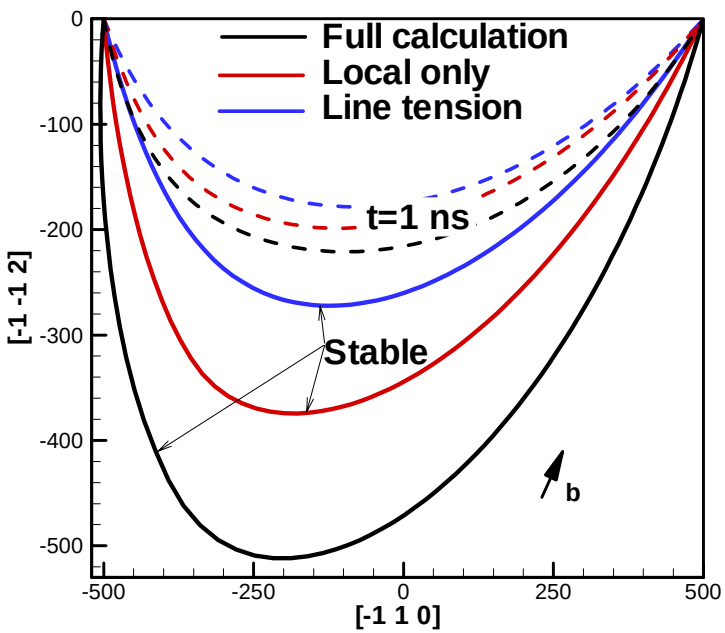
Anisotropic Ratio
$A=2C_{44}/(C_{11}-C_{12})$



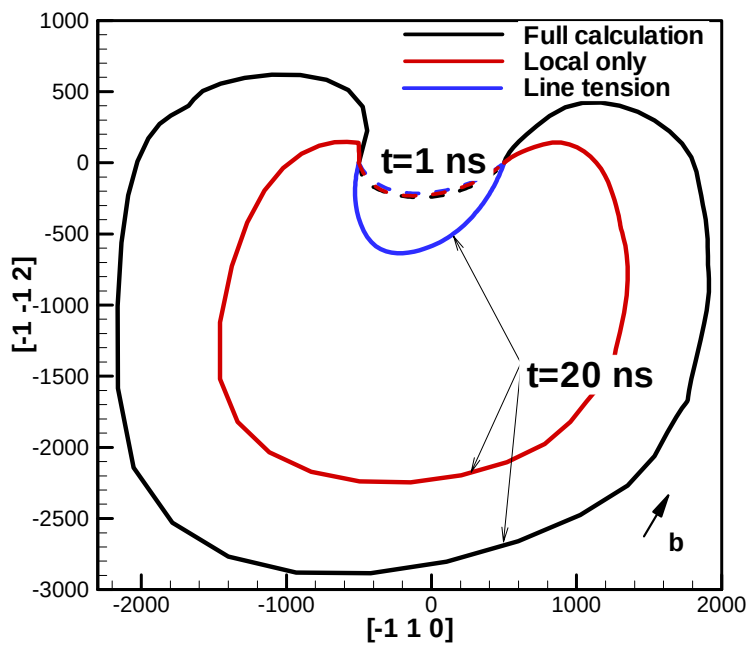


Stress **σ** (divided by $0.5(C_{11}-C_{12})b/R$)

Dislocation Dynamics in Anisotropic Materials

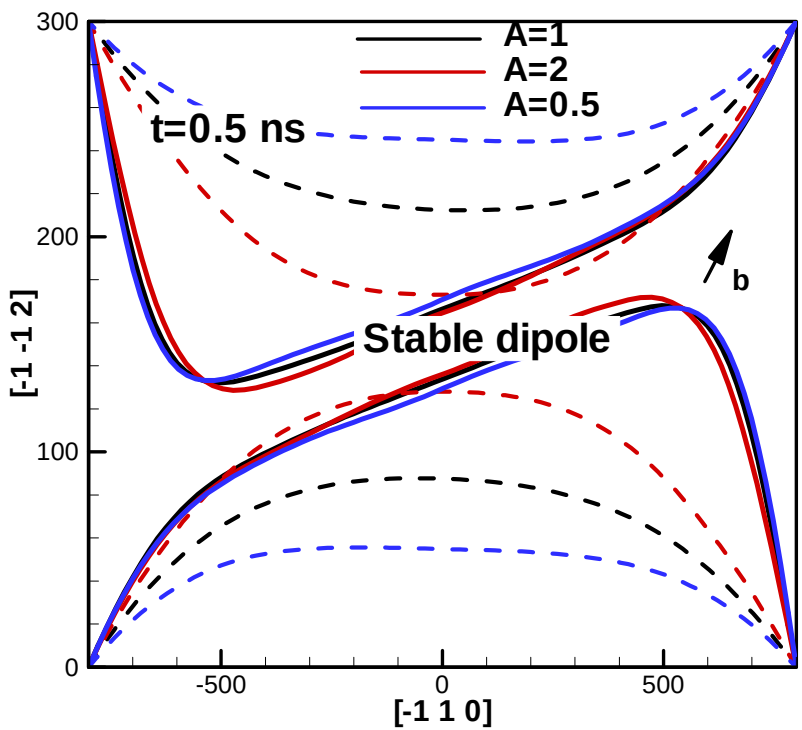


Isotropic A=1



Anisotropic A=0.5

Dislocation Dynamics in Anisotropic Materials



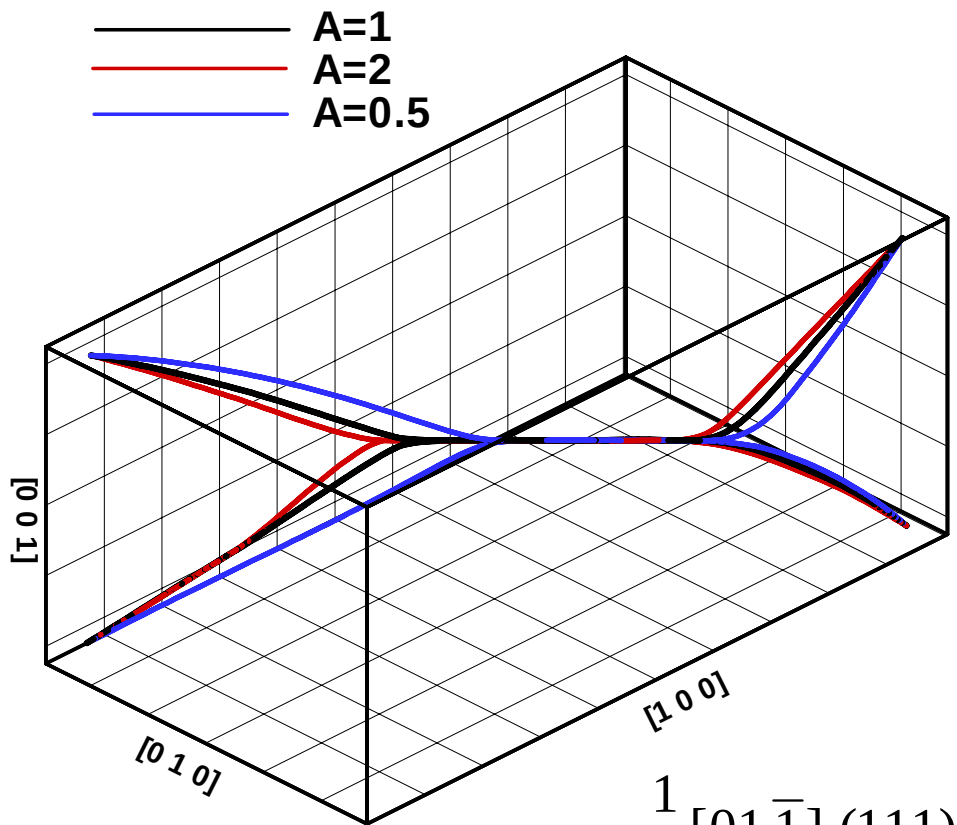
$$\mathbf{b} = \frac{1}{2}[\bar{1}01]$$

Parallel plane (111) seperated

$$h = 25\sqrt{3}a$$

No applied load

Dislocation Dynamics in Anisotropic Materials



$\frac{1}{2}[01\bar{1}]\,(111)$ **and** $\frac{1}{2}[101]\,(11\bar{1})$

Dislocation Interaction with Inclusions

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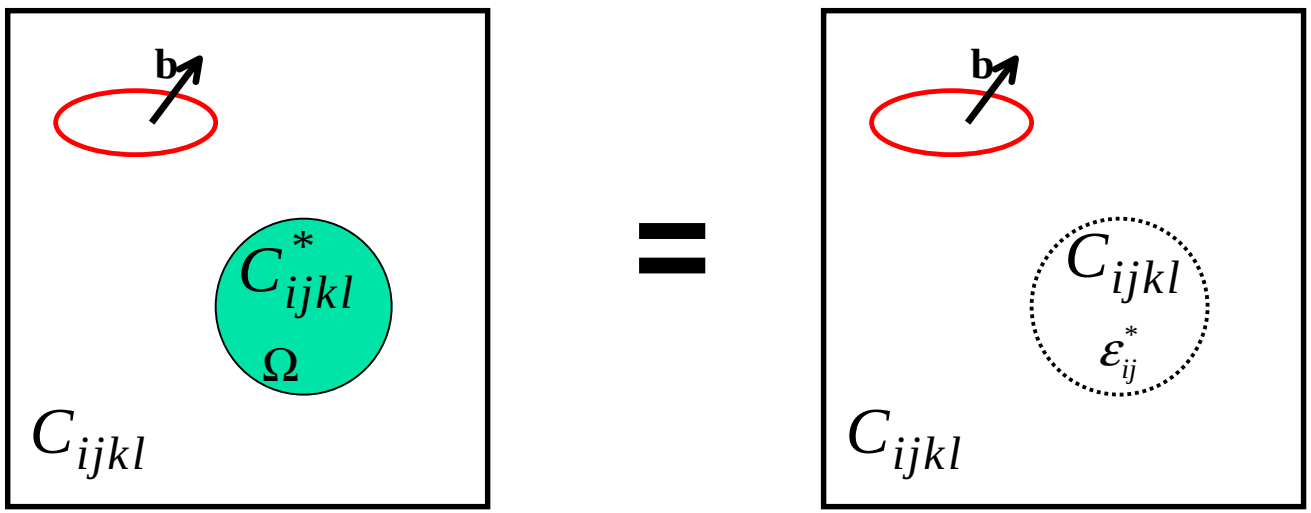
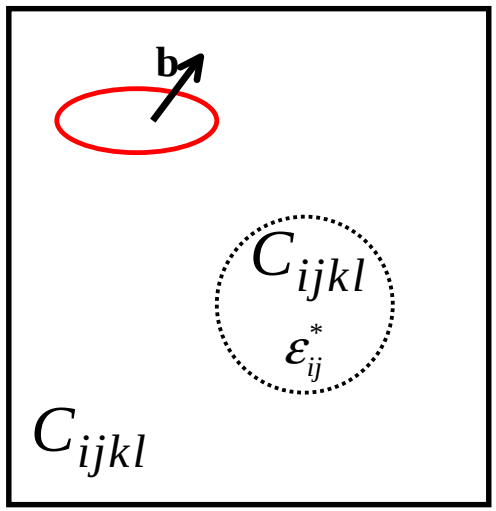
Dislocation Loops Interacting with Heterogeneous Inclusions



$$\varepsilon^*_{ij} = -[S_{ijkl} + (C^*_{ijmn} - C_{ijmn})^{-1} C_{mnkl}]^{-1} \varepsilon^d_{kl}$$

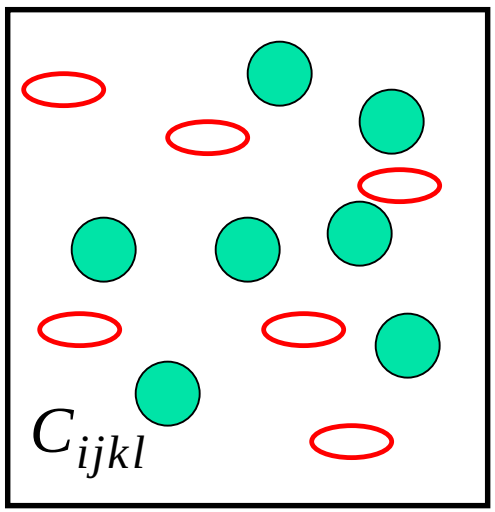
Dislocation Loops Interacting with Heterogeneous Inclusions



$$\sigma_{ij}(\boldsymbol{x}) = \sigma^d_{ij}(\boldsymbol{x}) + \sigma'_{ij}(\boldsymbol{x})$$

$$\sigma'_{ij}(\boldsymbol{x}) = C_{ijkl}\bar{G}_{klmn}(\boldsymbol{x})\varepsilon^*_{mn}$$

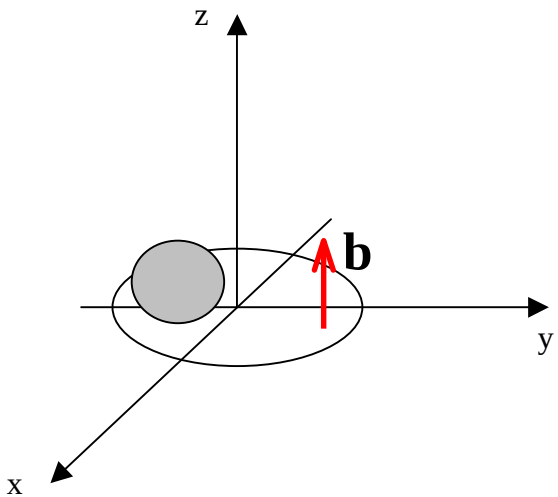
Dislocation Loops Interacting with Heterogeneous Inclusions



$$\sigma_{ij}(\boldsymbol{x}) = \sigma_{ij}^{d-total}(\boldsymbol{x}) + \sum_{m} \sigma'_{ij}(\boldsymbol{x}) | \sigma_{ij}^{d-total}(\boldsymbol{x})$$

$$\sigma_{ij}^{d-total}(\boldsymbol{x}) = \sum_{n} \sigma_{ij}^{d_n}(\boldsymbol{x})$$

Dislocation Loops Interacting with Heterogeneous Inclusions



Dislocation Loop: **R=100 b**

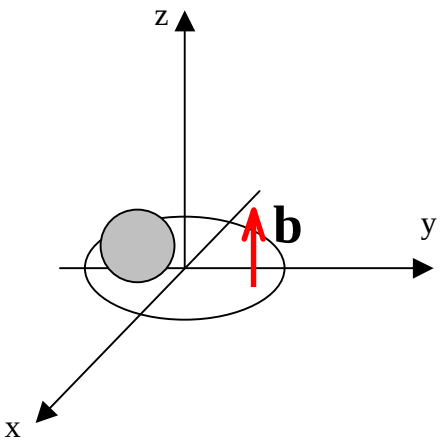
Particle: **r=20 b**

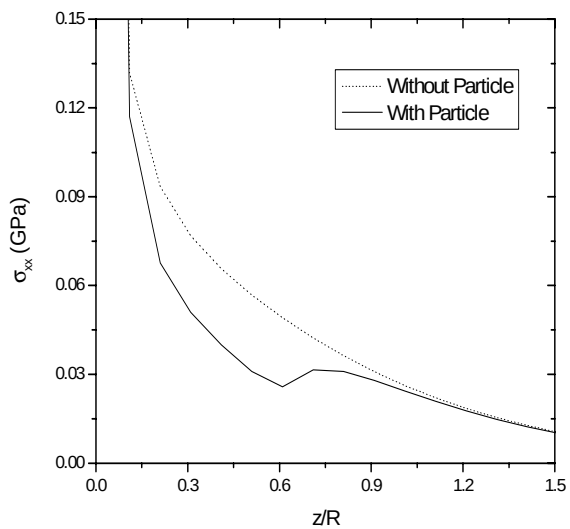
Particle center: **(R, 0, 0.4R)**

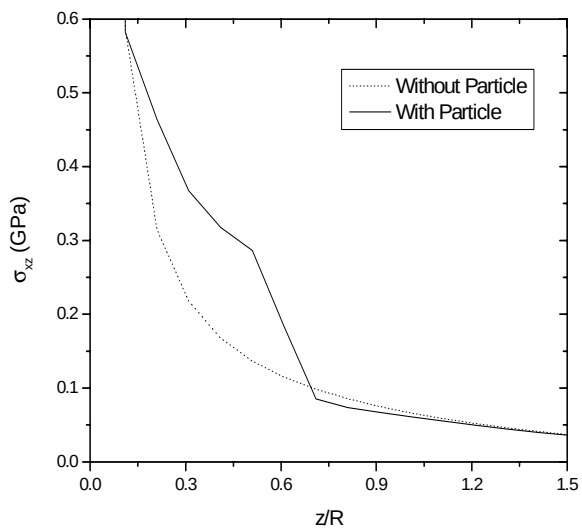
Constants of Materials: E_m**=73 GPa,** ν_m**=0.33**

E_p**=485 GPa,** ν_p**=0.20**

Dislocation Loops Interacting with Heterogeneous Inclusions







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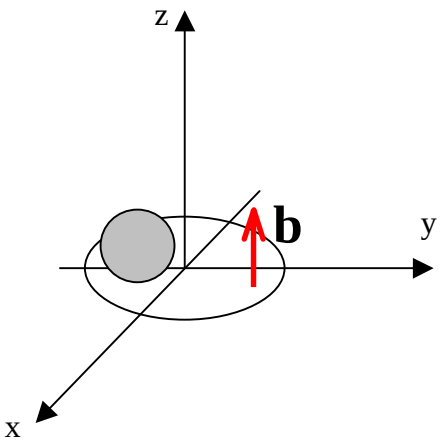
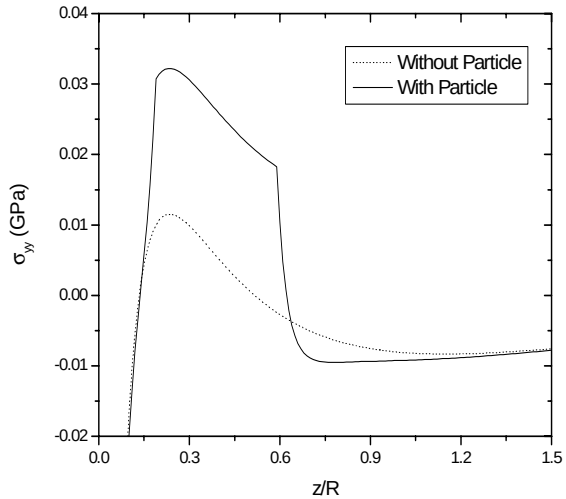
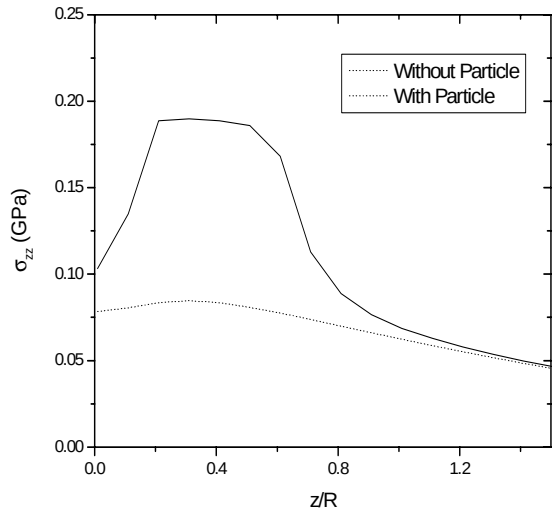
Dislocation Loops Interacting with Heterogeneous Inclusions







Dislocations in Thin Films

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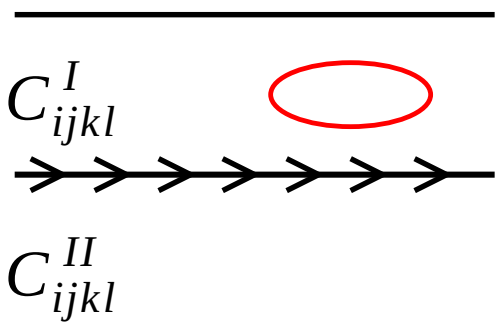
Elastic Fields of Dislocation Loops in the Film-Substrate Systems

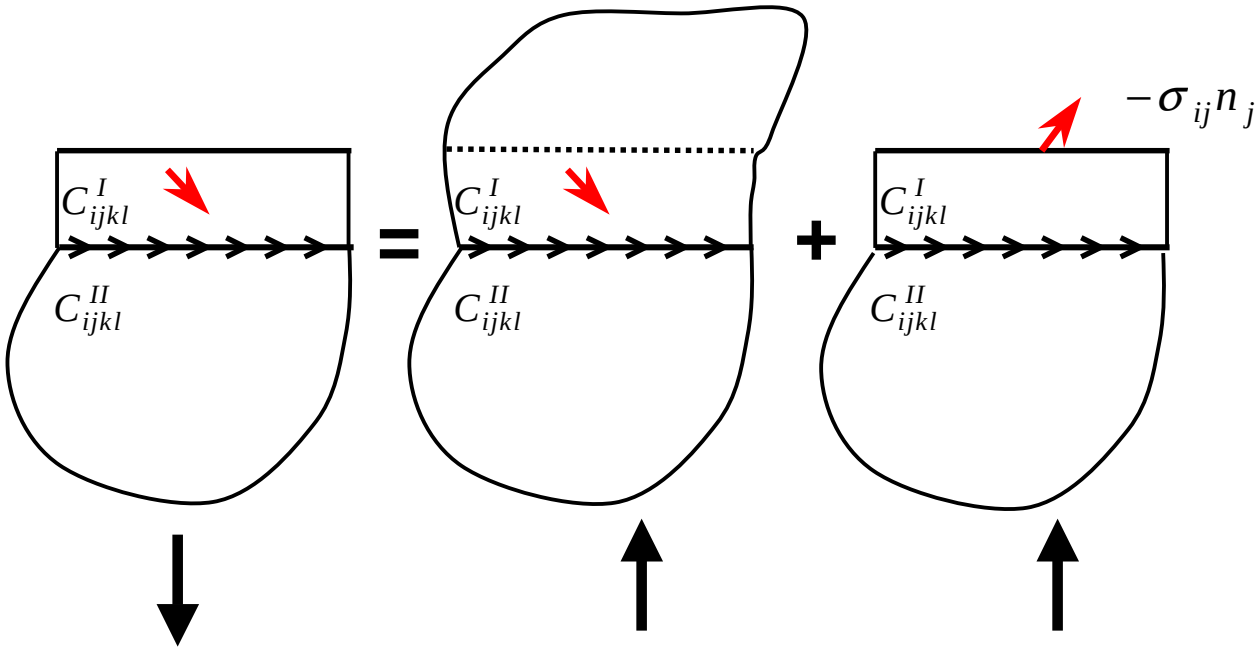


$$\sigma_{ij}(\boldsymbol{x}) = C_{ijkl} u_{k,l}(\boldsymbol{x})$$

$$u_m(\boldsymbol{x}) = -\int_{\partial V} b_i n_j C^{I}_{ijkl} \frac{\partial}{\partial x_l} G_{km}(\boldsymbol{x}', \boldsymbol{x}) dA$$

$$G_{km}(\boldsymbol{x}', \boldsymbol{x}) = ?$$

Elastic Fields of Dislocation Loops in the Film-Substrate Systems



$G_{km}(x', x)$

Rongved Solution

Integral Transforms

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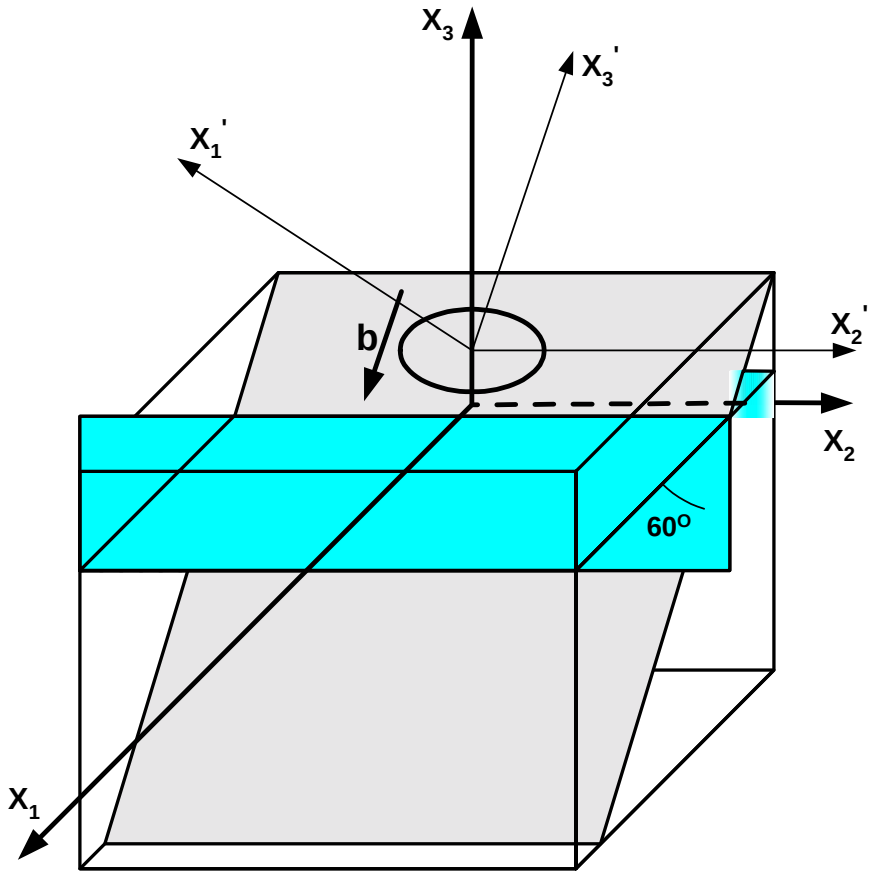
Elastic Fields of Dislocation Loops in the Film-Substrate Systems



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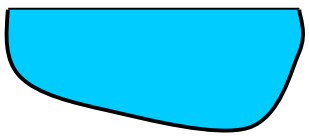
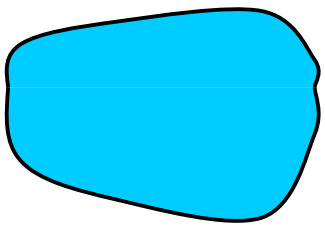
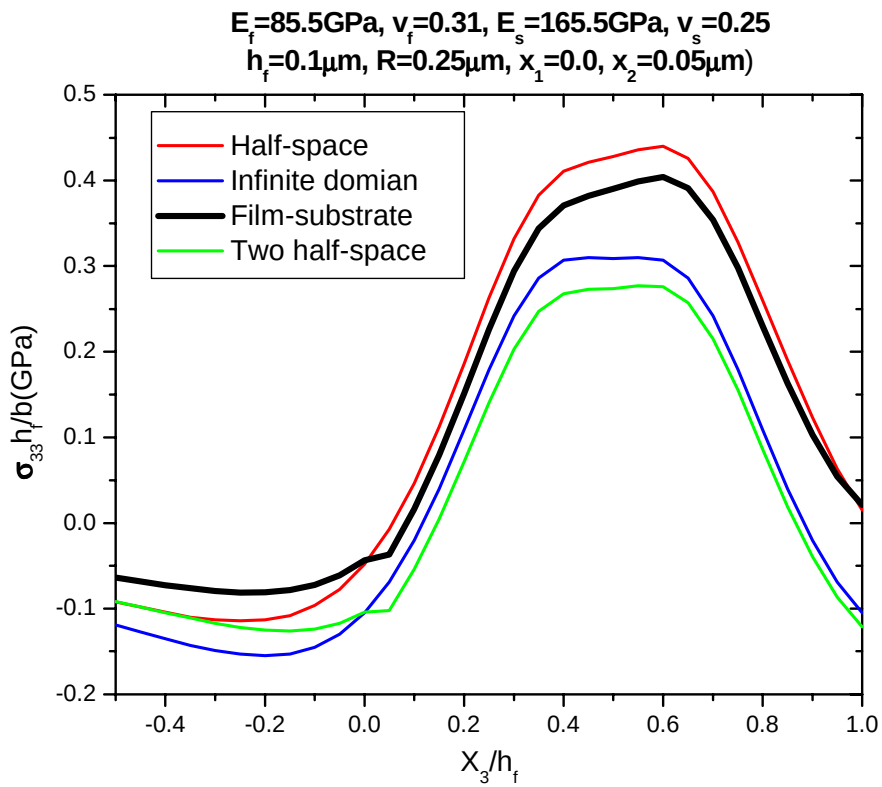
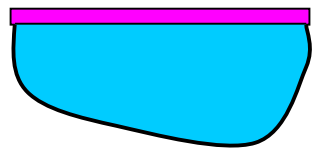


Half-space

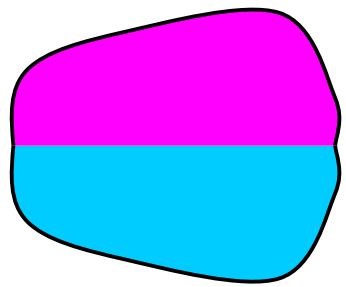


Infinite domain





Film-substrate



Two half-space

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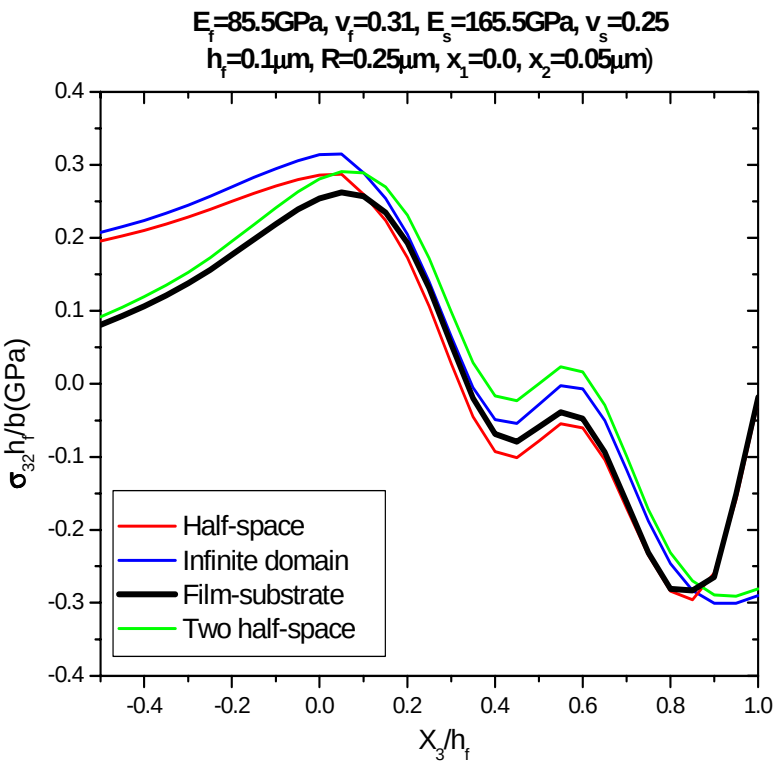
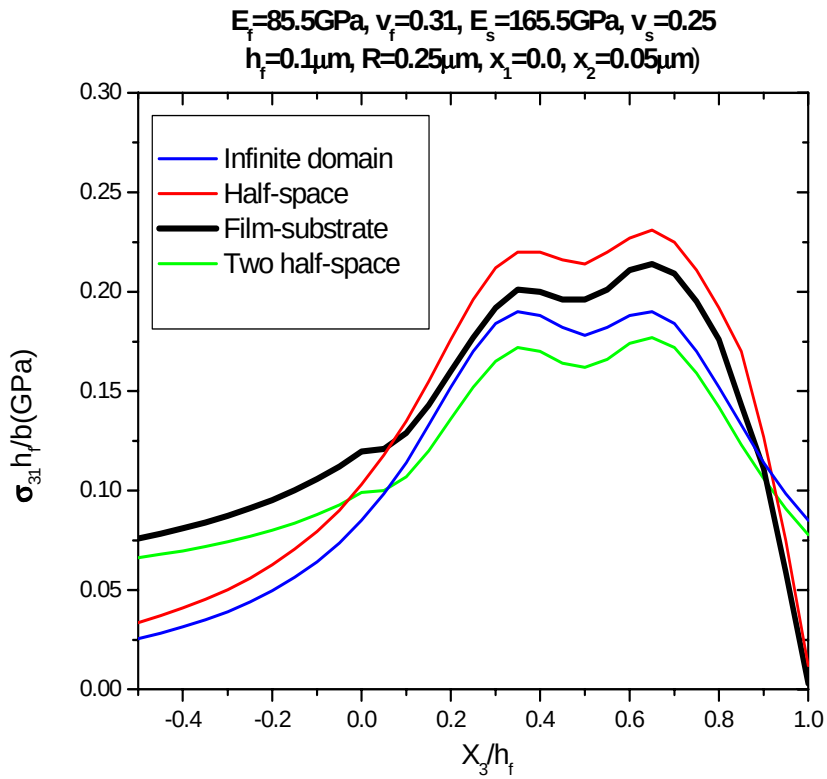
Elastic Fields of Dislocation Loops in the Film-Substrate Systems





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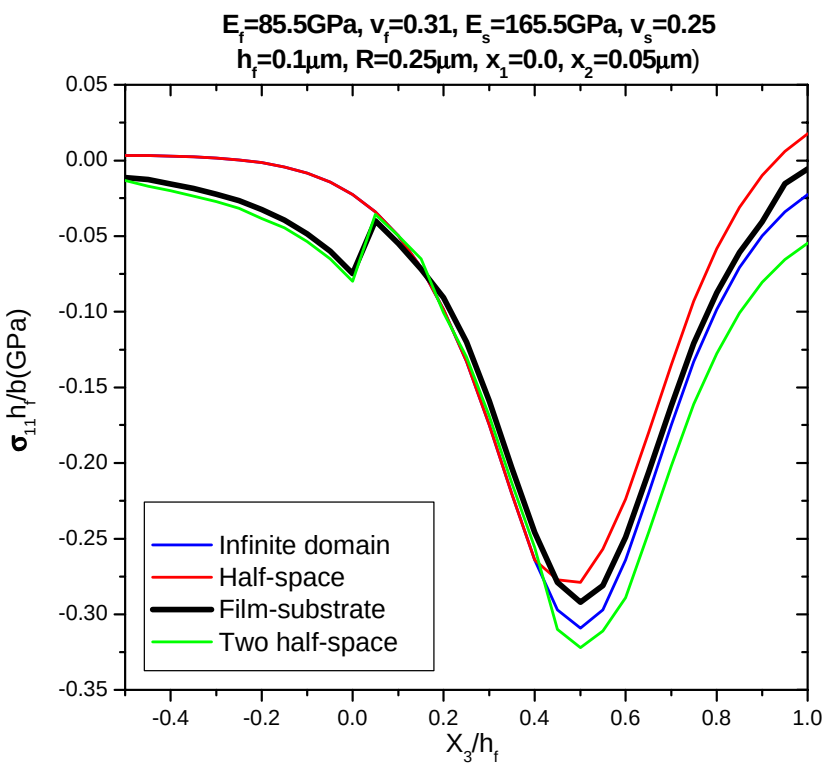
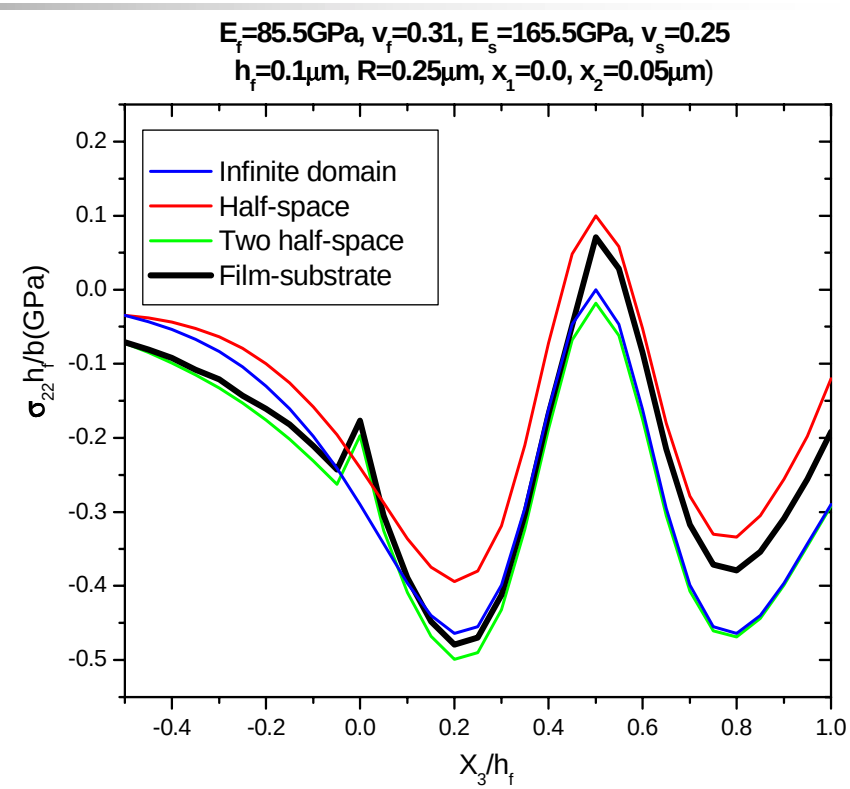
Elastic Fields of Dislocation Loops in the Film-Substrate Systems





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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)