LARGE-SCALE DISLOCATION DYNAMICS SIMULATIONS

for

COMPUTATIONAL DESIGN OF SEMICONDUCTOR THIN FILM SYSTEMS

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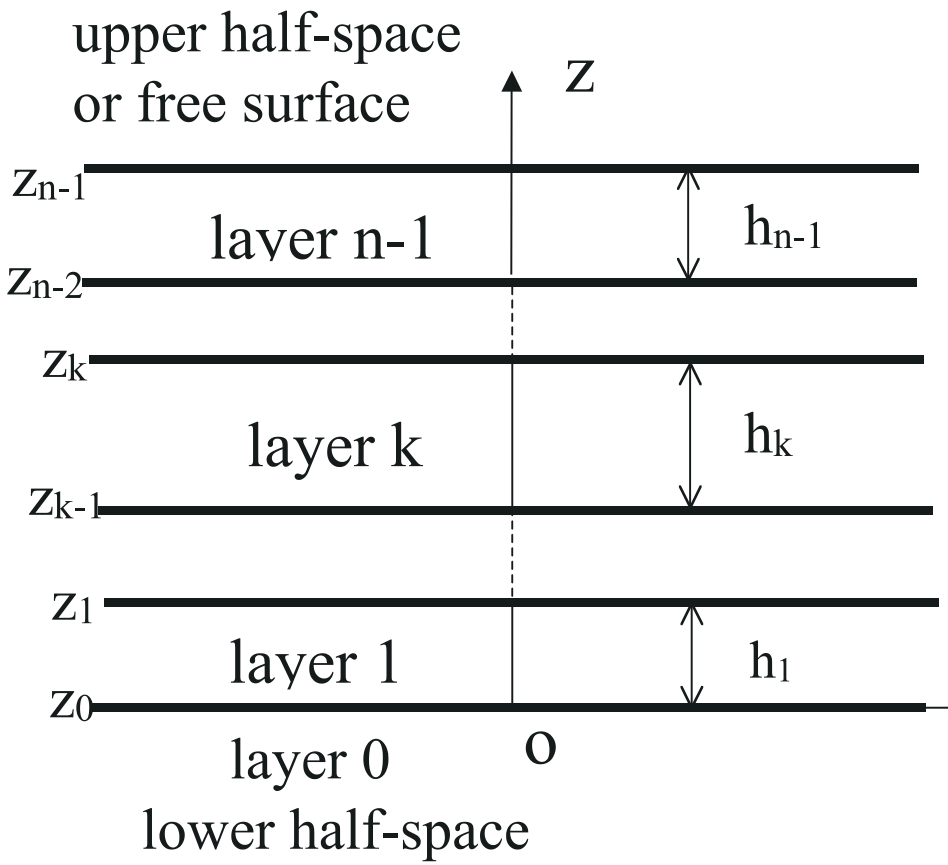
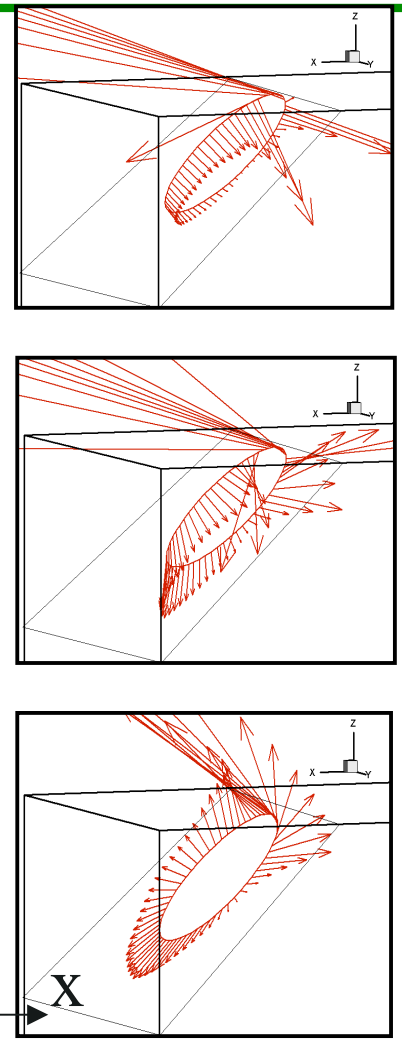
Project Objectives

- (1) Investigate single and collective dislocation interaction phenomena in anisotropic materials, which determine plasticity and failure of semiconductor devices.
- (2) Multiscale coupling of the parametric dislocation dynamics with the finite element
- (3) Develop unique software on parallel, scaleable computer clusters to simulate the collective behavior of topologically complex line defects.
- (4) Apply the developed software to investigate key dislocation mechanisms.
- (5) Large-scale simulation and optimization of semiconductor material systems.

Motivation: FEM+DD Superposition is Difficult

Many Thin Film Applications Require Mutilayers of Anisotropic Materials (Poly, or single crystal)





10a from z = 10000a boundary
scale factor = 1

50a from z = 10000a boundary
scale factor = 10

250a from z = 10000a boundary
scale factor = 10

Figure 5.4.2.3: Image force distributions for a 2000a radius loop at different distances from the z=10000a boundary. Scale factors as indicated.

Dislocation in Anisotropic Materials

The field of a dislocation loop in a non-homogeneous solid:

$$u_i(\mathbf{x}) = -\int_S C_{jlmn} b_m \frac{\partial}{\partial x'_l} G_{ji}(\mathbf{x}', \mathbf{x}) n_n(\mathbf{x}') \mathrm{d}S(\mathbf{x}')$$

$$\sigma_{ij}(\mathbf{x}) = -C_{ijkl}(\mathbf{x}) \int_S C_{pqmn}(\mathbf{x}') b_m \frac{\partial^2}{\partial x_l \partial x'_q} G_{pk}(\mathbf{x}', \mathbf{x}) n_n(\mathbf{x}') \mathrm{d}S(\mathbf{x}')$$

They are determined by using 2D Fourier transformation method:

$$\tilde{f}(\xi_1, \xi_2, x_3) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x_1, x_2, x_3) e^{\mathbf{i}\xi_\alpha x_\alpha} \mathrm{d}x_1 \mathrm{d}x_2$$

Where $G^{ji}(\mathbf{x}', \mathbf{x})$ are the Green's functions in a multilayer materials.

Dislocations in Anisotropic Multilayer Materials

The expression of Green's function is:

$$\tilde{\mathbf{G}}(\xi_1, \xi_2, x_3; \mathbf{x}') = e^{\mathsf{i}\xi_\alpha x'_\alpha} \left[\mathbf{i}\eta^{-1} (\bar{\mathbf{A}} < e^{-\mathsf{i}\bar{\mathsf{p}}\eta x_3} > \mathbf{V} + \mathbf{A} < e^{-\mathsf{i}\mathsf{p}\eta x_3} > \mathbf{W}) \right]$$

with p_i and $\mathbf{A}$ being the eigenvalues and eigenmatrix of

$$[\mathbf{Q} + p_i \mathbf{R} + \mathbf{R}^T) + p_i^2 \mathbf{T}] \mathbf{a}_i = 0$$

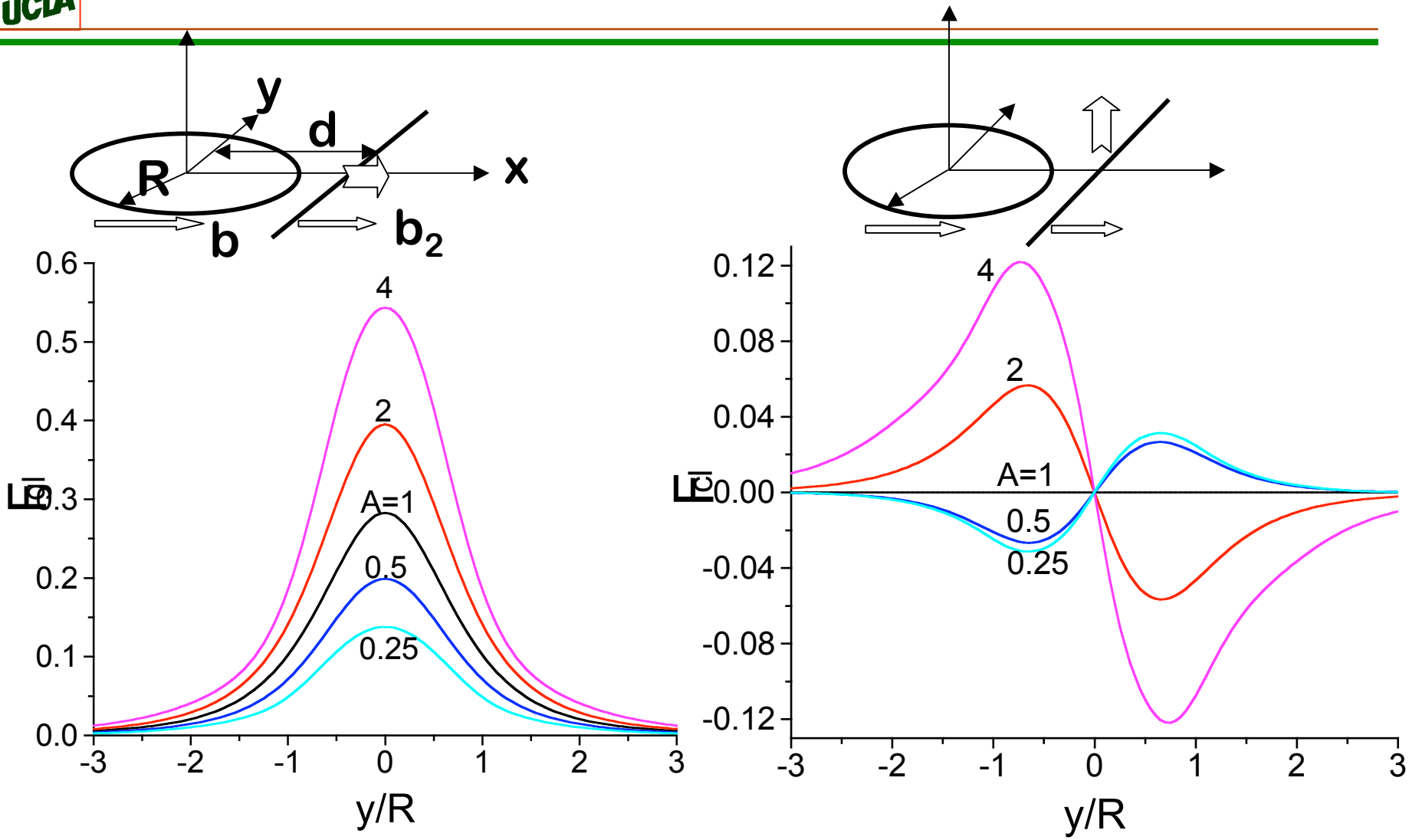
The out-of plane stress $\mathbf{t}$ and in-plane stress $\mathbf{s}$:

$$\tilde{\mathbf{t}}(\xi_1, \xi_2, x_3; \mathbf{x}') = e^{\mathsf{i}\xi_\alpha x'_\alpha} \left[(\bar{\mathbf{B}} < e^{-\mathsf{i}\bar{\mathsf{p}}\eta x_3} > \mathbf{V} + \mathbf{B} < e^{-\mathsf{i}\mathsf{p}\eta x_3} > \mathbf{W}) \right]$$

$$\tilde{\mathbf{s}}(\xi_1, \xi_2, x_3; \mathbf{x}') = e^{\mathsf{i}\xi_\alpha x'_\alpha} \left[(\bar{\mathbf{C}} < e^{-\mathsf{i}\bar{\mathsf{p}}\eta x_3} > \mathbf{V} + \mathbf{C} < e^{-\mathsf{i}\mathsf{p}\eta x_3} > \mathbf{W}) \right]$$

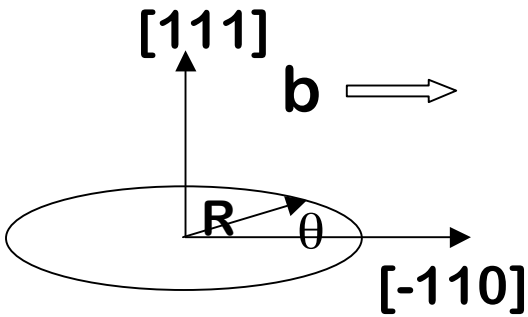
Using surface/interface conditions, Green's functions are determined in the transformed domain.

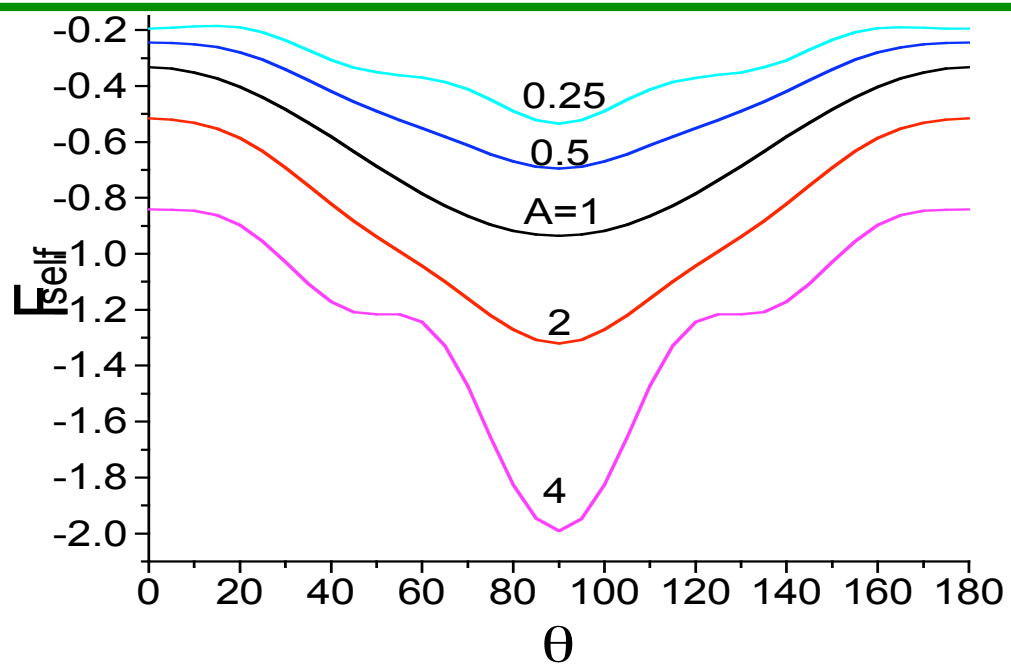
Peach-Koehler Force Distributions

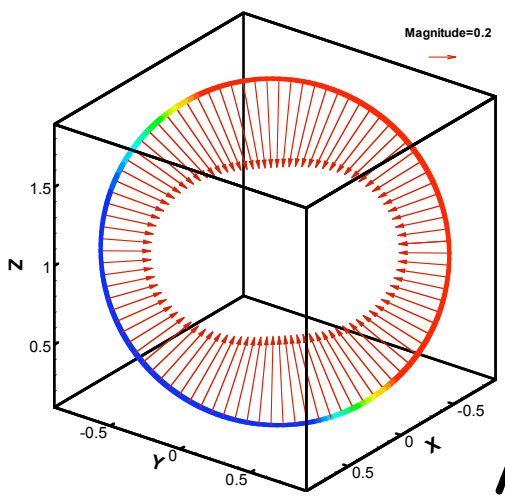


Forces divided by $0.5(C_{11}-C_{12})bb_2/R$, d=1.5R

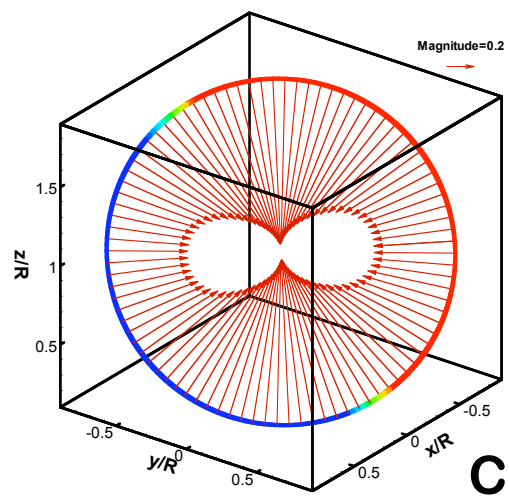
Self-Force Distributions





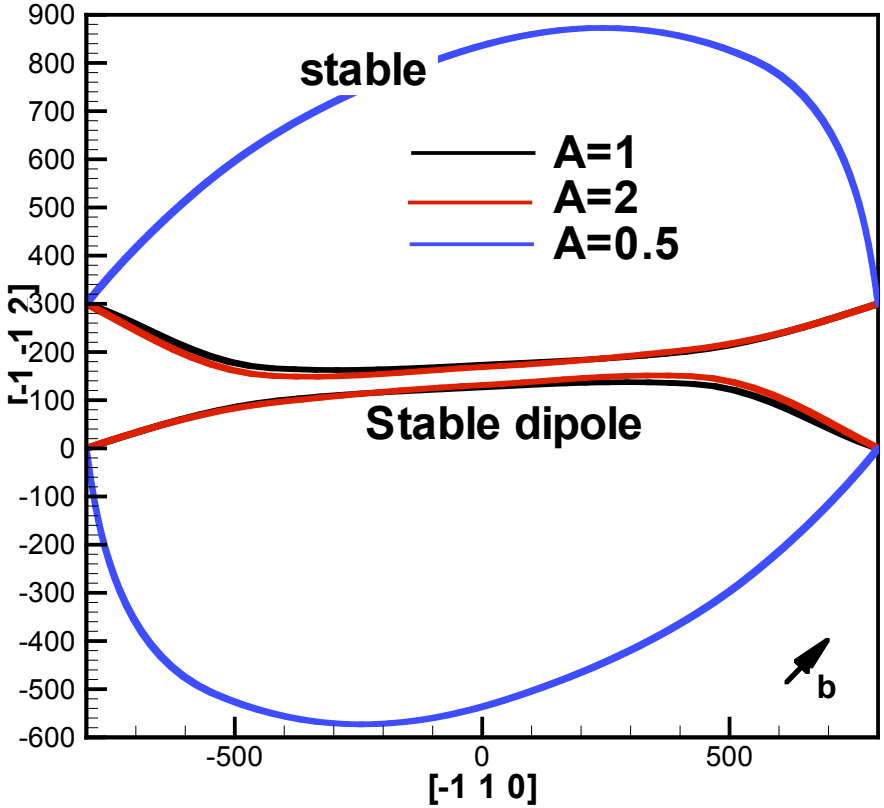


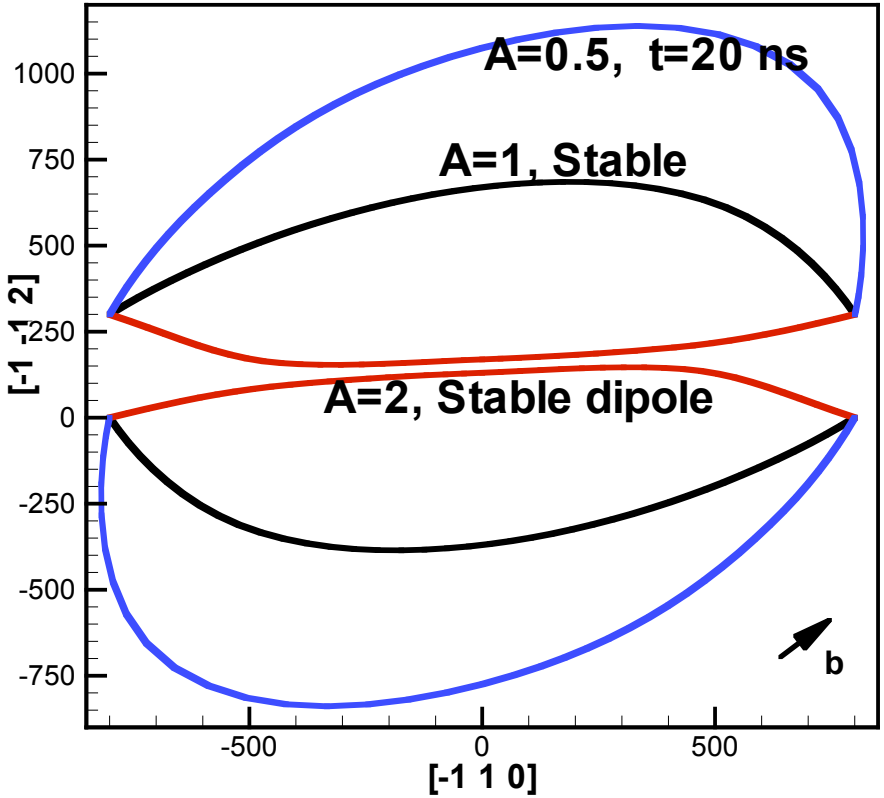
Al (A=1.21)



Cu (A=3.21)

Dislocation Dynamics
-Dipole Breakup





σ_{11}/μ=0.1%

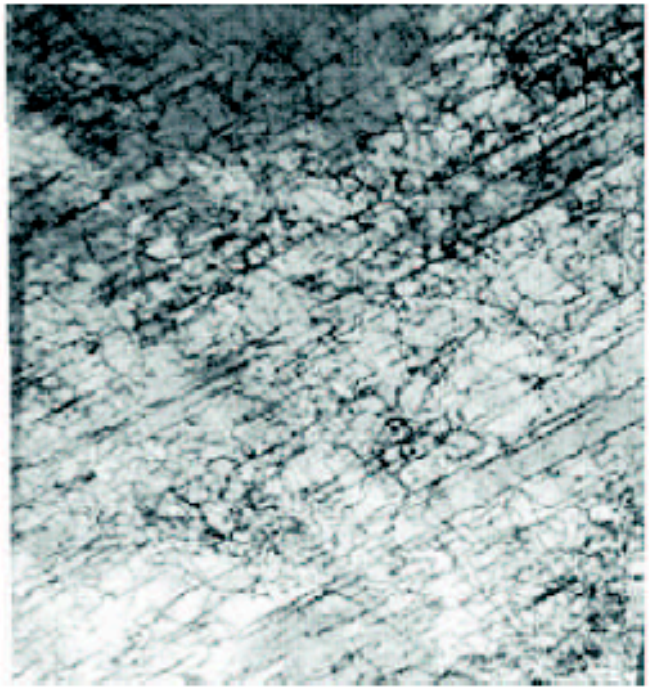
(Resolved shear stress is 0.04%)

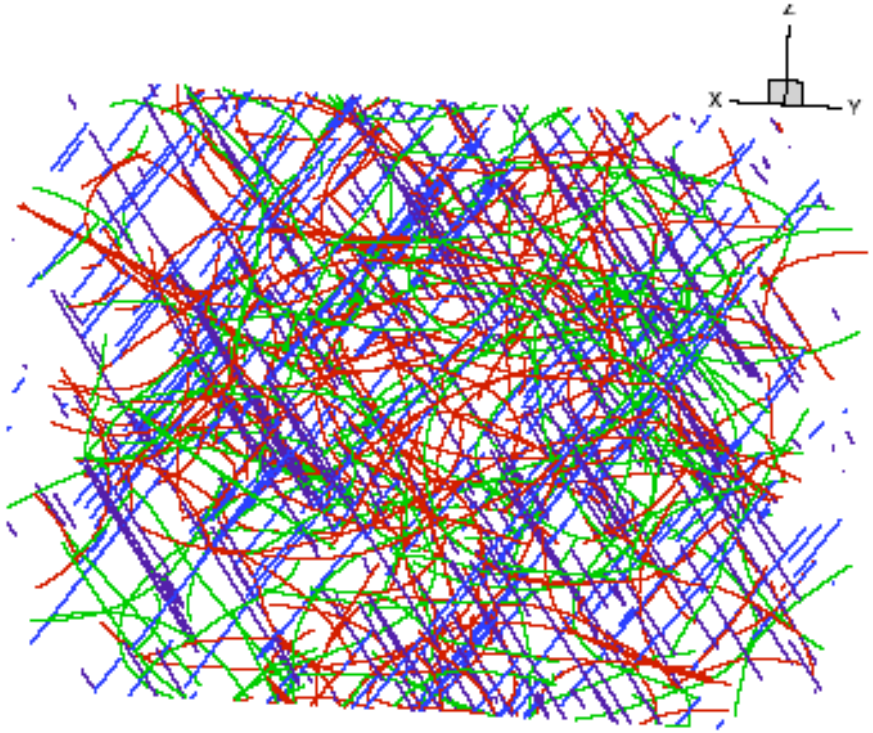
σ_{11}/μ=0.12%

(Resolved shear stress is 0.05%)

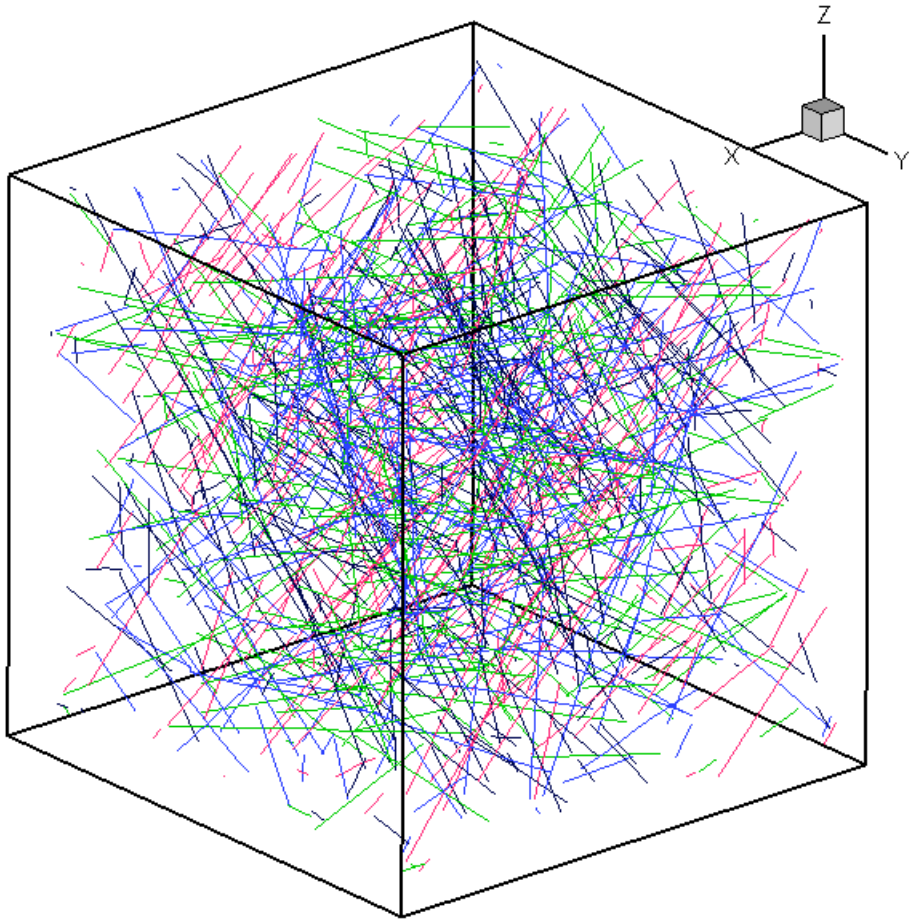
($\mu=(C_{11}-C_{12})/2$)

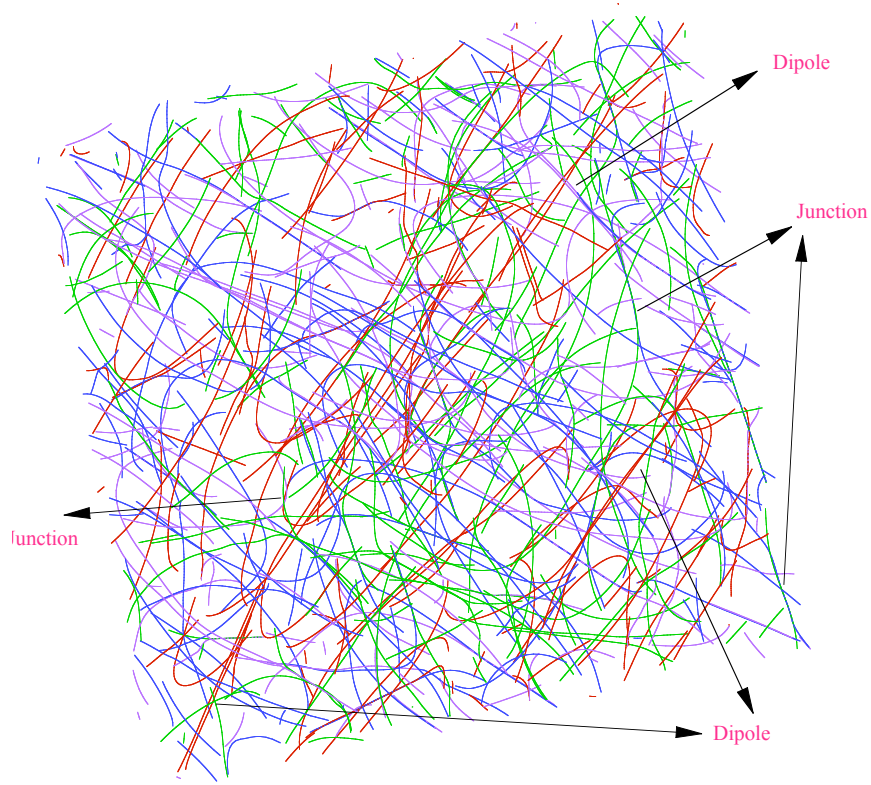
Results of Large Scale Simulation (cont.)



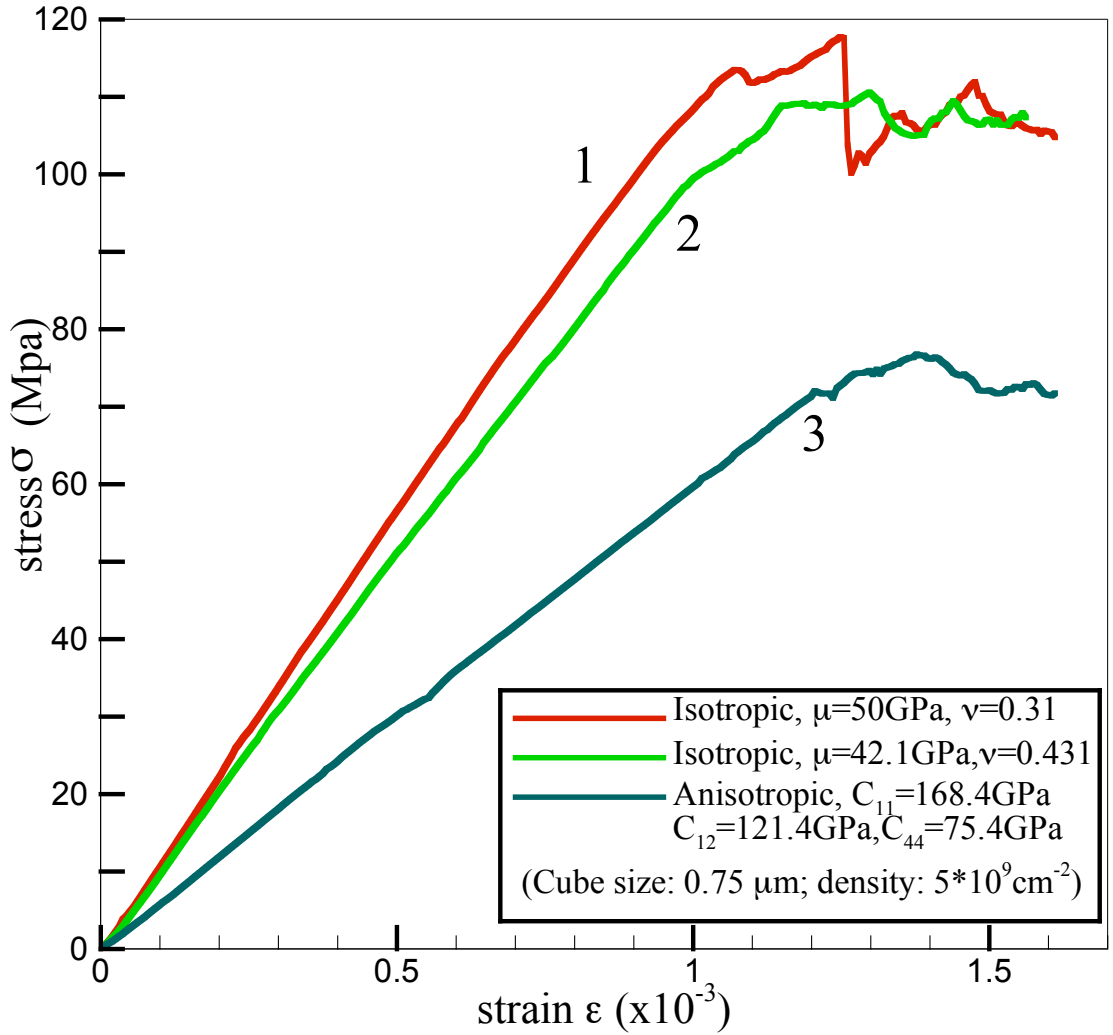


Results of Large Scale Simulation (cont.)



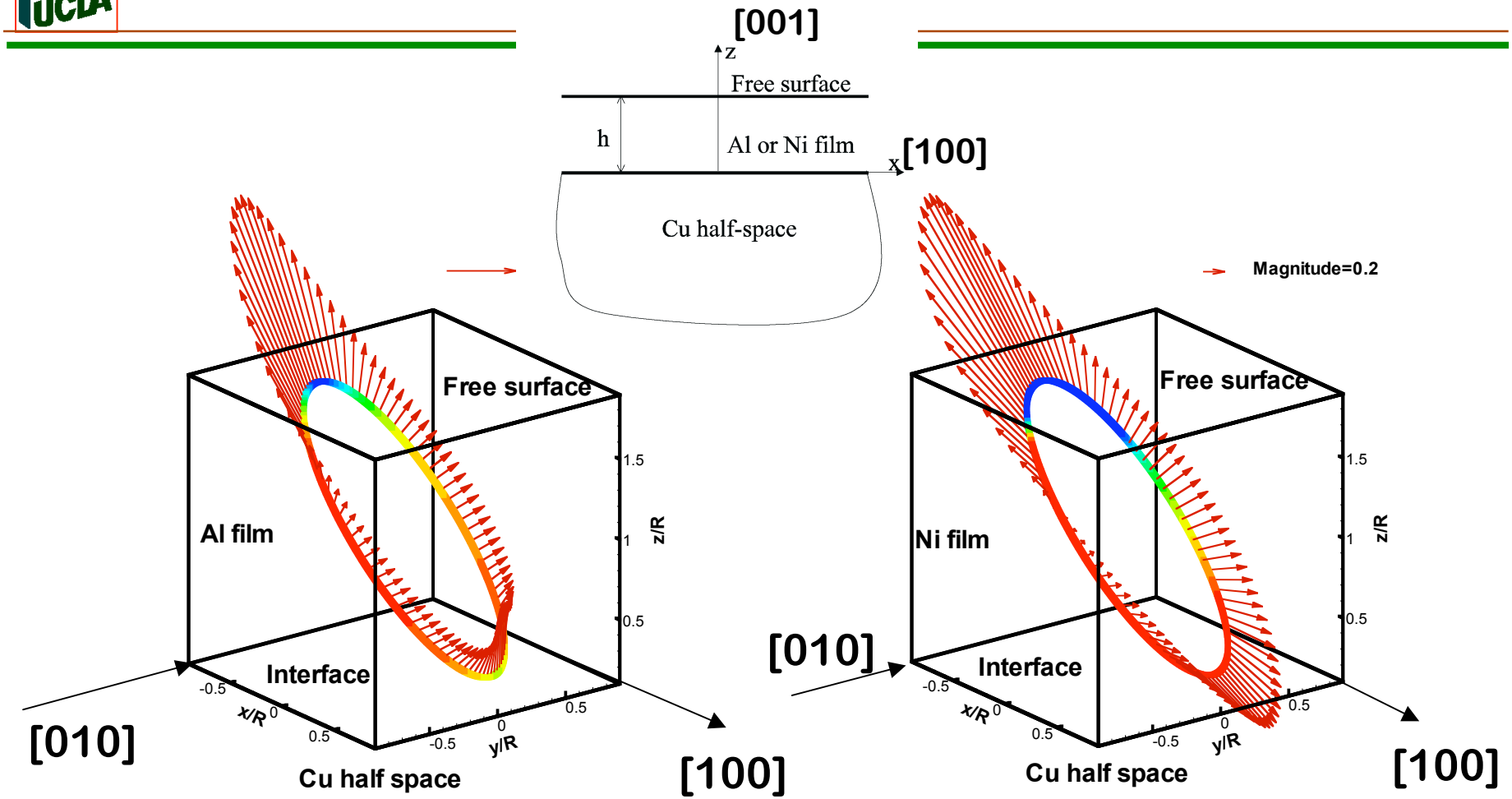


Strain Hardening in Cu



The stress field of dislocation loop in a thin film

- Peach-Koehler force due to interface



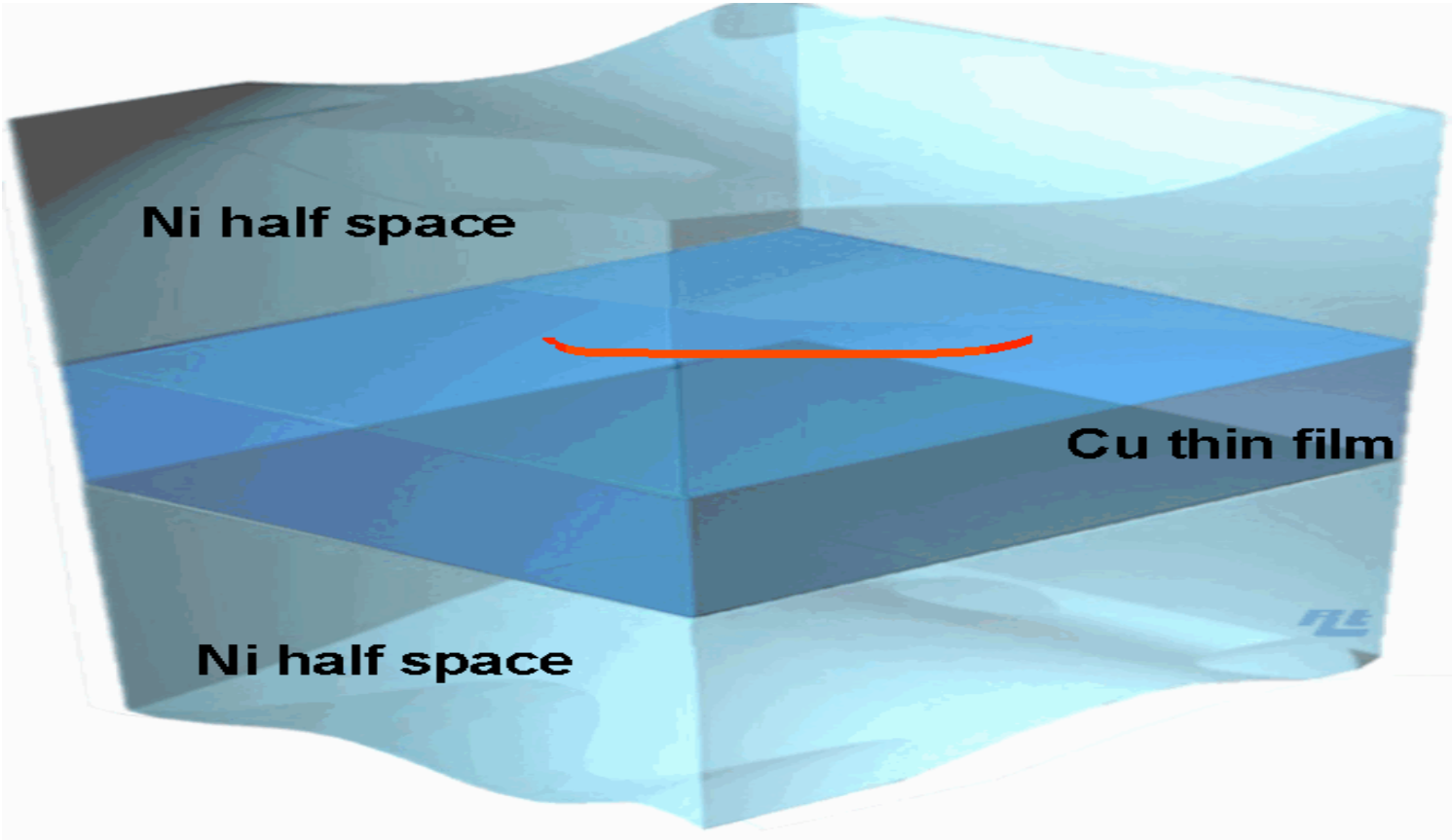
Al (film)-Cu (half space)

Ni (film)-Cu (half space)

Dislocation Motion with Interface Image Forces, ~ 30 nm < h < ~ 200 nm

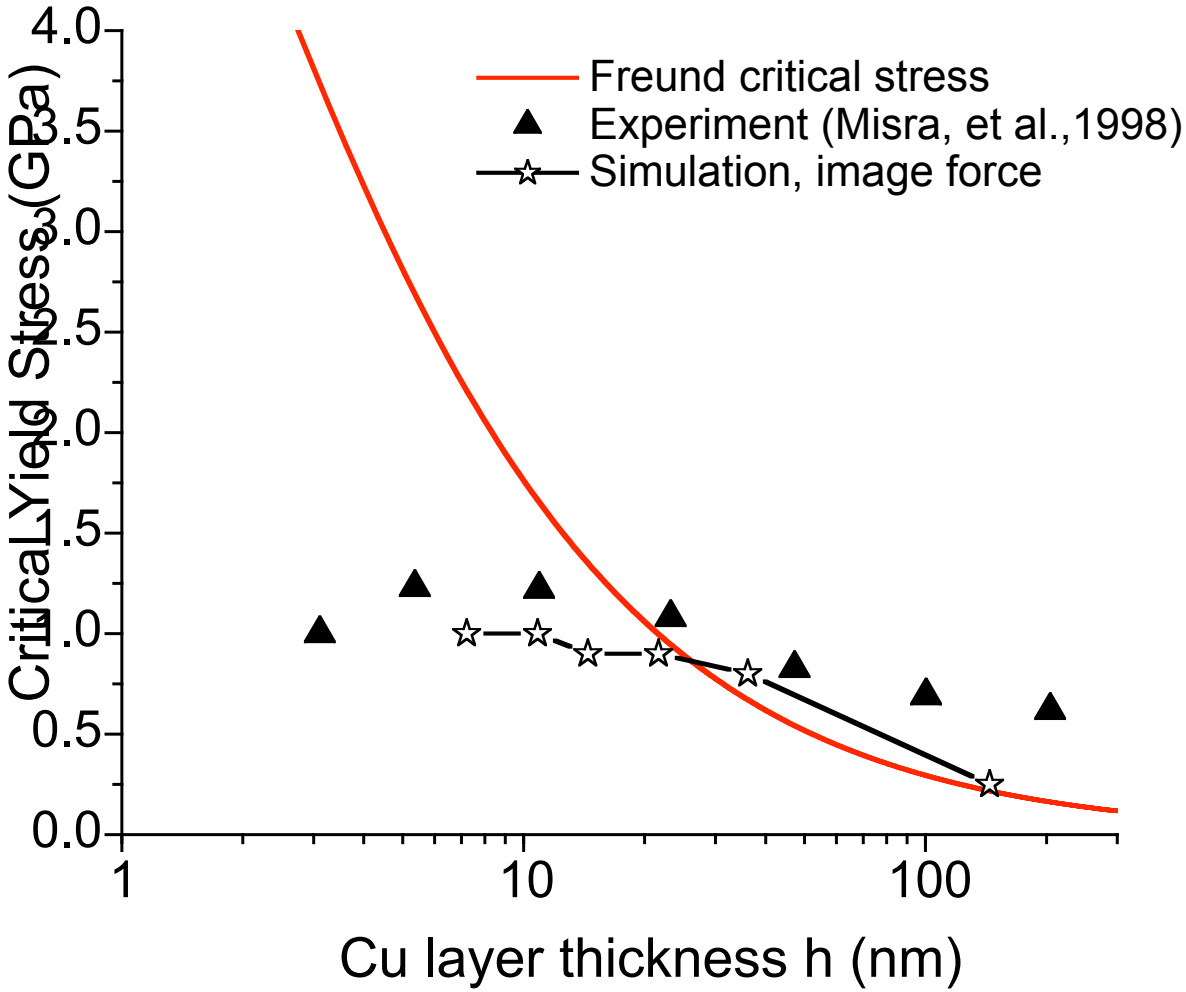
Critical Stress= 250 MPa

Film thickness, h=144nm

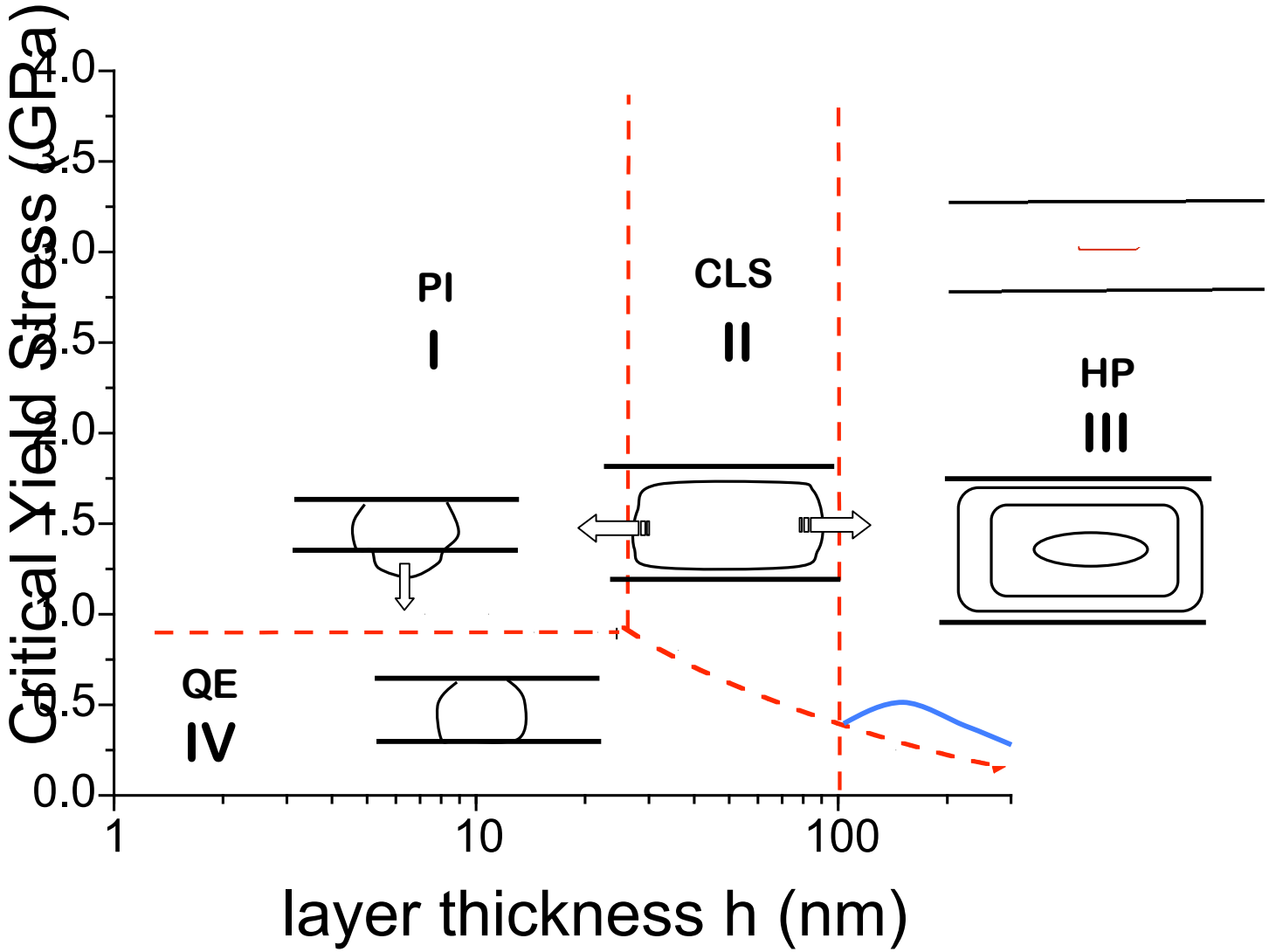


Above critical stress - Biaxial stress=280MPa

Critical Stress with Anisotropy & Image Forces



Deformation Modes in Multilayer Thin Films



Conclusions

- Elastic anisotropy results in unexpected effects (e.g. dislocation climb, dipole & F-R source stability).
- Larger values of the anisotropy ratio (A) results in an "equivalent" larger self-force.
- Equivalent isotropic elastic constants do not result in equivalent strain hardening.
- A method has been established to satisfy all interface & free surface B.C's in anisotropic thin films.
- Loops develop climb forces near interfaces.
- Good agreement with experiments on nano-indentation.

Publications & Activities

- **1.** X. Han, N. M. Ghoniem and Z. Wang**, "**Parametric Dislocation Dynamics of Anisotropic Crystals," Phil Mag**., Vol. 83, Nos. 31–34**, 2004.
- 2. N.M. Ghoniem, E. Busso, and N. Kioussis, "Multiscale modelling of nanomechanics and micromechanics: an overview," Phil Mag., **Vol. 83, Nos. 31–34**, 3475–3528, 2004.
- 3. J. Huang, N.M. Ghoniem*y* and J. Kratochv, "On the Sweeping Mechanism of Dipolar Dislocation Loops Under Fatigue Conditions, MSMSE, 2004.
- *4. Zhiqiang Wang, Rodney J. McCabe,Nasr M. Ghoniem, Richard LeSar, Amit Misra; and Terence E. Mitchel, "*Dislocation Motion in Thin Cu foils: A Comparison Between Computer Simulations and Experiment, " Acta Mater., 2004.
- 5 Nasr M. Ghoniem, and Nicholas Kioussis. "Hierarchical Models of Nano and Micro-Mechanics," Chapter in Encyclopedia of Nano Science & Technology, American Publishers, In Press.