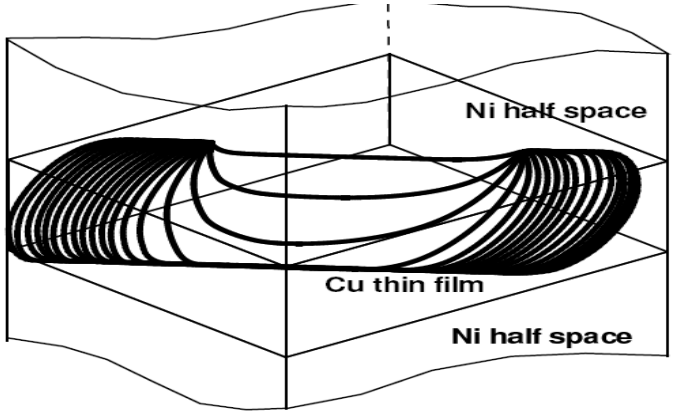
Large-scale Dislocation Dynamics Simulations for Computational Design of Semiconductor Thin Films

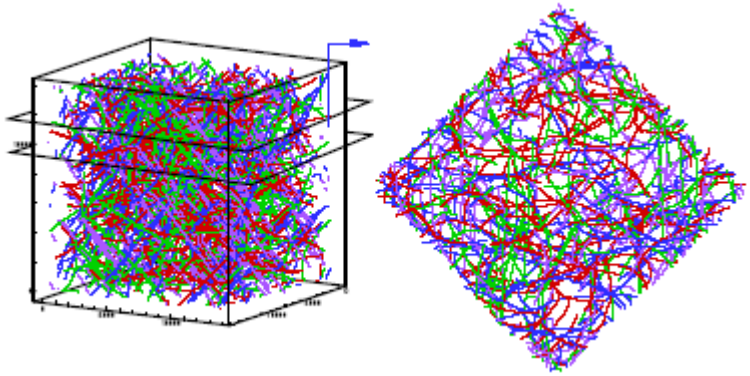
Nasr M. Ghoniem, University of California, Los Angeles, DMR-0113555

- We developed parallel computer software, based on discrete dislocation dynamics, which predicts deformation and failure of sub-micron semiconductor microelectronic thin films. The developed software is used to design desired mechanical properties of semiconductor thin film-substrate materials for nano- and micro-applications.

- The interaction forces between dislocations and free surfaces or interfaces in multilayer thin films have been determined. Our work extends the concept of the *Kohler barrier* in 2-D, and shows that the interface force depends on the relative ratio of elastic moduli of neighboring layers, the dislocation shape, the number of interactin adjacent layers, and layer thicknesses.

- The deformation modes of very thin films have been completely determined.





Top: Confined dislocation motion for h=144 nm under applied biaxial stress = 280 MPa. Each line corresponds to a time increment of 0.1 ns. **Bottom:** Simulated dislocation microstructure in Cu interconnect single crystal.

Publications: (1) N. M. Ghoniem, H. Huang, E. Busso, and N. Kioussis, "Multiscale Modeling of Nano- and Micro-Mechanics: an Overview," *Phil. Mag. A*, **83 (31–34)**, 3475–3: (2003).
(2) X. Han, N.M. Ghoniem and Z. Wang,"Parametric Dislocation Dynamics of Anisotropic Crystalline Materials," *Phil. Mag. A.*, **83 (31–34)**, 3705–3721, (2003).
(3) N. M. Ghoniem and N. Kioussis, "Hierarchial Models of Nanomechanics and Micromechanics," *Encyclopedia of Nanoscience and Nanotechnology, American Scientific Publisher;* ,**in Press**, (2004).
(4) X. Han and Nasr M. Ghoniem, "Stress Field and Interaction Forces of Dislocations in Anisotropic Multilayer Thin Films," *Phil. Mag., **In Press,** 2004.*

Large-scale Dislocation Dynamics Simulations for Computational Design of Semiconductor Thin Films

Nasr M. Ghoniem, University of California, Los Angeles, DMR-0113555

Education:

Two undergraduate students: Jon Sugar and William Newsome, and two graduate students: Qiang Hu and Zhiqiang Wang contributed to this research. The Ph.D. thesis of Qiang Hu is on the design of self-assembled quantum dots, as a result of extending the original software, developed by Xueli Han (Post-doctoral fellow) and the P.I. The research has contributed to a new seminar course at UCLA (MAE259B: Advanced topics in Solid Mechanics). The course covers many topics in nano- and micro-mechanics, and some of the material is derived from this NSF-supported research.

Outreach:

(1) Two high school students: Ehab El-Naga and Erol Gurol, were trained in Professor Ghoniem's group.

(2) Professor Ghoniem taught an NSF-sponsored short course on nano-mechanics to Latin American Scientists and students in Rio de Janeiro, Brazil.

(3) One Ph.D. student, Voijta Minarik, and his advisor, professor Jan Kratochvil, spent one month collaborating in Professor Ghoniem's Lab.