Department of Civil Engineering and Engineering Mechanics
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Continuum and Continuum-Atomistic Simulations of Dislocations

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Mesoscale and multiscale models of dislocations can provide useful insight into the mechanics of dislocations, an understanding of which is important for the improvement of the reliability of MEMS devices and to further our understanding of the mechanisms governing crystal plasticity. We will present a newly developed mesoscale continuum dislocation model based on the Extended Finite Element Method (XFEM) . In contrast to most existing models, which are based on the superposition of isotropic infinite domain solutions, the XFEM dislocation model is applicable to both large deformation problems and to anisotropic materials. Furthermore, the method is applicable to problems involving material interfaces, such as those that exist in thin films and MEMS devices.

Continuum-based dislocation models breakdown in the vicinity of the dislocation cores. Multiscale models of dislocations, where atomistic models are used near the dislocation cores are therefore attractive. Existing multiscale models of crystal plasticity suffer from a significant limitation - as these simulations progress, large regions of the simulation domain are converted from continuum to atomistics to accommodate the evolution of the dislocations. The number of atoms in existing multiscale models is proportional to the area of the slip surfaces which connect the dislocation lines. In the second part of our seminar, we will describe a new continuum-atomistic framework for modeling dislocations which allows one to retain atomic resolution in the near core region only. This framework significantly reduces the number of degrees of freedom because the number of atoms in the model is proportional to the length of the dislocations lines.

April 14, 2009 (Tuesday)

3:00 - 4:00 p.m.
Room 627, Mudd

`http://www.civil.columbia.edu/~ling/seminar`