

Mechanism Based Modeling and Simulation in Nanomechanics *NSF NIRT Grant 0103257*

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Project Objective

Crystalline materials display a strong size dependence in mechanical behavior over a scale that extends from nanometers to microns. Understanding the fundamental mechanisms of this dependence has important implications for design and fabrication of structures and devices in nanotechnology. The objective of this project is to develop mechanism-based multiscale computational modeling and simulation that can be used to study the mechanical behavior of crystalline materials from the nanometer to the micron scale. In particular, the role of discrete dislocation nucleation, motion, and interaction is investigated. The nanoindentation technique is also used to probe the mechanical response of materials as well as to validate computational modeling and simulation. In addition, we develop continuum analyses that directly incorporate atomistic models in order to study the nanoscale mechanical properties of the material. To demonstrate this effective continuum-atomistic linkage, we study the mechanical properties of nanotubes, where the mechanical properties are directly controlled by atomic-scale processes.

Research Progress

We have developed a nanoindentation technique that can be used to probe the mechanical response of materials from the nanometer to the micron scale. Our experiments on metal single crystals focus on the fundamental mechanisms of initial elastic-plastic transition at the nanoscale. The experimental results indicate that mechanical behavior of crystalline materials deviates from conventional continuum mechanics models and the deformation of the materials exhibits discrete behavior (Fig. 1, Ref. 1). The analysis of experimental results indicates that this behavior is related to dislocation nucleation under nanoindentation.

In collaboration with national laboratories, direct atomistic simulation has also been used to validate and understand the discrete plastic deformation under nanoindentation (Fig. 2; Ref. 1, 2). The simulation reveals that nucleation of dislocations may occur beneath the nanoindenter, where it is unaffected by surface imperfections.

A combined atomistic and continuum model based on the Peierls-Nabarro dislocation model is developed to study dislocation nucleation in crystals. This approach allows us to incorporate atomic information into continuum approach to obtain the saddle point configurations of embryonic dislocations in three-dimensional configurations (Fig. 3; Ref. 3-5). The study of dislocation nucleation under an idealized nanoindentation further confirms that the

size dependence and the discrete behavior of plastic deformation under nanoindentation are related to the physical process of dislocation nucleation and interaction (Fig. 4).

Our continuum analyses based on atomistic models have demonstrated excellent predictive power of nanoscale mechanical and thermal properties, as well as coupled electrical property with mechanical deformation (Fig. 5, 6; Ref 5-7). We have studied single wall carbon nanotubes and established that, without any parameter fitting, our nanoscale continuum model agrees very well with the atomistic models in the study of pre-deformation energy, elastic modulus, fracture strain, critical strain for defect nucleation, electrical conductance change due to mechanical deformation, and the thermal expansion coefficient.

Relevance to Nanotechnology

Successful design and manufacturing of nanoscale devices and systems must involve concerted efforts in understanding the unique mechanical behavior of materials at the nanoscale. Our research is aimed at developing effective computational modeling and simulation that can predict the mechanical behavior of crystalline materials and structures based on the fundamental dislocation mechanisms. The detailed analysis of dislocation nucleation, motion, and interaction will have high academic and industrial impacts because their broad implications on mechanical, electrical, and optical behavior of crystalline materials. Typical examples include brittle versus ductile behavior of materials, growth of high quality strained heteroepitaxial semiconductor layer structures for high speed electronics and optoelectronic, defects in stress driven self-assembly or evolution of quantum structures on the surface, and nanoscale engineering crystalline materials with superior mechanical properties. Our research also pushes forward the envelope of mechanics that will extend from the continuum level, through the domain of discrete dislocation plasticity to the atomistic scale. The framework of continuum-atomistic linkage will have far-reaching significance in nanoscale engineering analysis.

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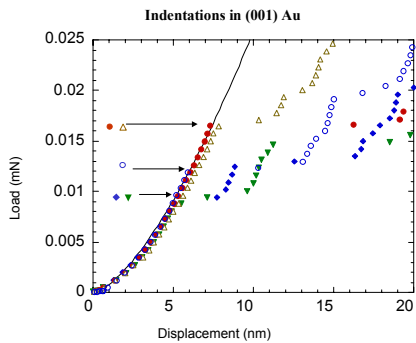


Fig. 1 Discrete plastic deformation in nanoindentation experiments.

Atomistic simulation of load drop due to the emission of a dislocation loop under indentation

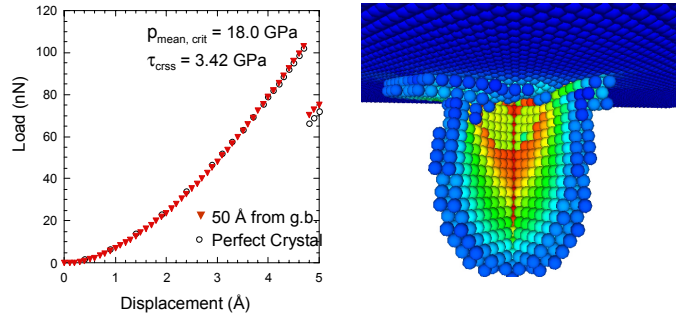


Fig. 2 Atomistic simulation of nucleation of a dislocation loop under nanoindentation

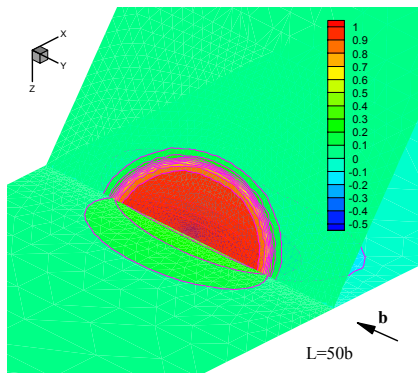


Fig. 3 Nucleation of a dislocation loop from the surface (surface turned upside).

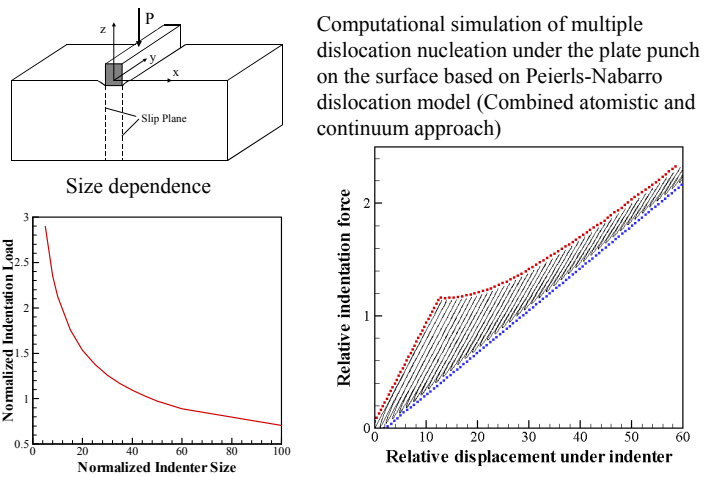


Fig. 4 Combined atomistic and continuum simulation of size dependence and discrete deformation in nanoindentation.

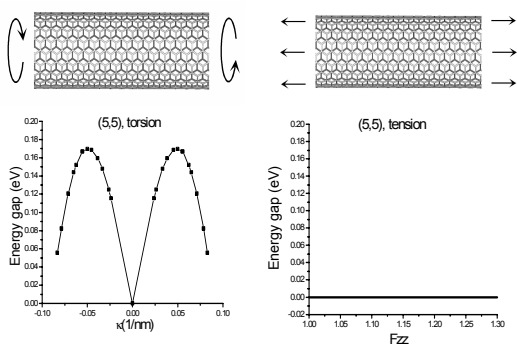


Fig. 5 Effect of mechanical deformation on electrical properties of carbon nanotube.

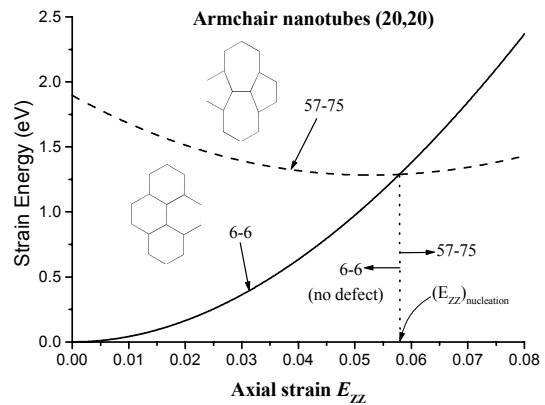


Fig. 6 Critical stress for defect nucleation in carbon nanotube.