

Invited Speaker : Professor **Boris I. Yakobson**, Departments of Mechanical Engineering and Materials Science, Department of Chemistry, Smalley Institute for Nanoscale Science and Technology, Rice University

Title :

Atomic mechanics of nanotubes: Elasticity, yield, superplasticity?

Date & Time: 23 March 2007, 13:00~14:30

Place: The University of Tokyo, Engineering Building II, 3rd Floor, Room 232

Abstract:

Mechanics at the nanoscale blends the notions and intuition of mechanical engineering with the fundamentally different aspects of solid state physics and quantum chemistry [1]. Through our studies of nano-tubes and wires, we have encountered the situations when such interpenetration can be very useful, but can also be misleading. The stability and structure of nearly 1-dimensional wires of silicon and metals contrast to the "no-surface" structure of the nanotubes. The particular atomistic mechanisms of relaxation have been identified, with the distinctly different sensitivity to the temporal and thermal conditions: the single bond flip-rotations or the brittle unzipping through a series of lattice-trapped states. Combination of static barrier computations with the probabilistic approach of transition state theory allows one to compare the different channels of mechanical relaxation and to determine the strength limits as a function of time, symmetry, and temperature [2]. This leads to a construction of yield-strain map, for the tubes of different chirality, at various temperatures, and different load rate. Predictions and recent discoveries of superplasticity [3-4], and coalescence/welding-leading to nanofoams for possible hydrogen storage-will also be considered in atomistic detail.

[1] Yakobson and Smalley, American Scientist 85, 324-337, (1997).

[2] Dumitrica et al. Proc. Natl. Acad. Sci. 103, 6105-6109 (2006).

[3] "How evaporating nanotubes retain their perfection?" Ding et al. Nano Lett. (2007-02-16).

[4] "Pseudo-climb in superplastic nanotubes" Ding et al. Phys. Rev. Lett. 98, 075503 (2007).

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