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Theory of superplasticity and atomic relaxation in nanotubes and fullerenes FENG DING, KUN JIAO, YU LIN, MS&MS Dept., Rice University, JIANYU HUANG, Center for Integrated Nanotechnologies, Sandia National Laboratories, BORIS I. YAKOBSON, MS&MS Dept., Rice University, YAKOBSON TEAM, JIANYU HUANG COLLABORATION — Plastic relaxation of carbon nanotubes under tension and at high temperature have been described in terms of dislocation theory and with atomistic computer simulations. Now we show how the glide of pentagon-heptagon defects and a particular type of their pseudo-climb [1], with the atoms directly breaking out of the lattice, work concurrently to maintain the tube perfection. Derived force diagram quantifies the balance between these mechanisms, while simulations show both helical and longitudinal movement of the kinks. Mass reduction also represents a compelling problem [2], and we present a mechanism of high-temperature sublimation of carbon nanotubes and giant fullerenes [3]. It does not destroy their ordered makeup even upon significant loss of mass. The atoms depart to the gas phase from the pentagon-heptagon dislocation cores, while the bond disruption is immediately repaired, and the 5|7 seamlessly propagate through the lattice. This explains a broad class of unsettled phenomena when at high temperature or under radiation the nanotubes do not become amorphous but rather shrink in size nearly flawlessly. We also will present our recent [1] F. Ding, et. al., Phys. Rev. Lett. 98, 075503 (2007) [2] F. Ding, et. al., Nano Lett. 7, 681 (2007) [3] J. Huang, et. al., Phys. Rev. Lett. 99, 175503 (2007)

Feng Ding
MS&MS Dept., Rice University

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