Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Continuum description of defects in carbon nanotubes ELIF ERTEKIN, DARYL CHRZAN, University of California, Berkeley — Recently, indications of plastic deformation have been observed in carbon nanotubes: strain stiffening in nanotube torsional shafts and direct observations of kink motion to assist with elongation. These observations suggest the importance of defects, both their formation and dynamics, to nanotube mechanical properties. Remarkably, defect formation energies are not well–understood: formation energies of Stone–Wales defects (dislocation–like defects) vary by ≈ 3 eV, depending on the environment. Further, no attempt has been made to compute the total energies of dissociated Stone–Wales defects. To address these issues, we develop a continuum theory of defect formation in nanotubes based on the idea that the distortion field associated with the presence of a defect distribution is that which minimizes the elastic and curvature energies but is consistent with the topological constraints imposed by the defects. It makes no a priori assumptions about the defect strain fields, accounts for defect–defect interactions, and accomodates changes to the curvature and out–of–plane buckling. Formation energies of Stone–Wales defects in a wide variety of configurations are computed using total energy electronic structure methods and compared with the results of the continuum theory; the agreement is excellent, irrespective of defect arrangement. The result is an accurate and transferable continuum description of defect formation energies in carbon nanotubes.

Elif Ertekin
University of California, Berkeley

Date submitted: 18 Nov 2006 Electronic form version 1.4