Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Self-Healing of Divacancies in Carbon Nanotubes. SAVAS BERBER, University of Tsukuba, ATSUSHI OSHIYAMA, University of Tsukuba — We investigate the occurrence and reconstruction of divacancies in carbon nanotubes, and the electronic structure modification by defects using *ab initio* Density Functional calculations. Structure optimization calculations on both arm-chair and zig-zag defective nanotubes with diameters ranging from 4 Å to 9 Å reveals self-healing ability of defective nanotubes. Nanotube with ideal divacancy transforms into more stable structure by concerted formation of 2 new bonds, leaving no unsaturated bonds. Diameter dependence of reconstruction energy and formation energy of divacancies depend on the mechanism of strain distribution for particular orientation of the defect. Divacancy formation is a possible way to stabilize the tubes with high concentration of monovacancies. Band structure of relaxed defective tubes indicate that metallic tubes mostly keep their metallic character while semiconducting tubes may acquire metallic character due to appearance of additional energy levels inside band gap of perfect tube due to new bonds formed during healing process. Five membered rings in relaxed structure can be recognized by a raised profile in simulated Scanning Tunneling Microscope (STM) images, providing a detection tool. In addition, we explore thermal stability of defective nanotubes by elevating the temperature in Nosé-Hoover molecular dynamics simulations using a parametrized electronic Hamiltonian.

Savas Berber
University of Tsukuba

Date submitted: 28 Nov 2004 Electronic form version 1.4