Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The effects of 5-7 defects on the mechanical characteristics of carbon nanotubes intramolecular junctions and their influences on electronic properties WEN-JAY LEE, JEE-GONG CHANG, YENG-TSENG WANG, WAN-SHENG SU, National Center for High-Performance Computing, Tainan 741 — This study utilizes molecular dynamics simulations and first-principles techniques to investigate mechanical and electronic properties of the single-walled carbon nanotube (SWCNT) intramolecular junctions (IMJs). Results show that the mechanical behaviors are mainly affected by the diameter of thinner segment of two composed tubes, whereas are barely able to be influenced by the number of 5-7 defects in the interface region. With applied compression, the yielding stress and Young's modulus of the SWCNT IMJs are found to be strongly associated with the orientation of two contacted heptagon rings where their ordering values are vertical > tilted > parallel to the axial direction. Under applied tensile, a lowest value in the yielding stress and Young's modulus is found on the parallel status, but the other two reveal alternating relations. Moreover, the magnitude of the stress amplitude is proportional to the Young's modulus and yielding stress and the buckling location is shown to be dependence on different orientations of two contacted heptagon rings. Finally, our first-principles calculations indicated that the considered SWCNT (5,0)/(8,0) IMJs at a certain length with different distributions of 5-7 defects on the tube wall exhibit diverse electronic properties, such as the changes of the density of states and modulation of energy gap. With increasing length, the numbers of states near the Fermi level region increase significantly and the energy gap tends to shrink as well.

Wan-Sheng Su
National Center for High-Performance Computing, Tainan 741

Date submitted: 08 Nov 2011 Electronic form version 1.4