Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Deep levels in the band gap of the carbon nanotube with vacancy-related defects[1] GUNN KIM, N.C. State University, USA, BYOUNG WOOK JEONG, JISOON IHM, Seoul National University, Korea — We study the modification in the electronic structure of the carbon nanotube induced by vacancy-related defects using the first-principles calculation. Three defect configurations which are likely to occur in semiconducting carbon nanotubes are considered. A vacancy-adatom complex is found to bring about a pair of localized states deep inside the energy gap. A pentagon- octagon-pentagon topological defect produced by the divacancy is structurally stable and gives rise to an unoccupied localized state in the gap. We also discuss the character of partially- occupied localized state produced by a substitutional impurity plus a monovacancy.

[1]This work is supported by the SRC program (Center for Nanotubes and Nanostructured Composites) of MOST/KOSEF, the BK21 project of KRF and the MOST through the NSTP (grant No. M1-0213-04-001).

Gunn Kim
N.C. State University

Date submitted: 29 Nov 2005 Electronic form version 1.4