Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

First Principles Calculations for Destructive Deformation of Carbon Nanotubes by Oxygen Molecule TAKAZUMI KAWAI, YOSHIYUKI MIYAMOTO, NEC Corp. — It is well-known that carbon nanotube devices are significantly sensitive to ambient gas molecules such as oxygen molecules. Especially chemisorbed oxygen molecules have possibility to destruct carbon network and even destroy the devices. Then oxidation of carbon nanotubes is crucial for nano device application. On the other hand, the oxidation is very useful method to cut the cap structures or purify nanotubes by burning the defective nanotubes. Furthermore, some experimental results suggest that the chirality dependent oxidation of nanotubes. To understand the properties of oxidation, we focus on an initial process where the C=C bond is broken after the cyclo-addition of oxygen molecule on nanotube surface. The DFT-LDA calculations show that the diameter dependence and also the chirality dependence of reaction barriers to break the C=C bond. We will also discuss the effect of hole doping which would correspond to the oxidation process in solution.

Takazumi Kawai
NEC Corp.

Date submitted: 16 Nov 2006 Electronic form version 1.4