

# Molecular Dynamics Study of Phase Change of Water inside a Single-Walled Carbon Nanotube

Shigeo Maruyama

Dept. of Mech. Eng., The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

The phase change of liquid water to ice crystal inside a single-walled carbon nanotube (SWNT) was studied with molecular dynamics simulations. Water molecules were modeled with SPC/E potential and carbon-carbon interaction was expressed by Brenner potential. The carbon-water interaction was expressed with the Lennard-Jones function with the quadrupole interaction term. An SWNT with liquid water inside was initially kept in equilibrium at 300 K. Then, the carbon atoms were cooled at the constant cooling rate. The liquid to solid phase change for various cooling rates in a SWNT with various chiralities were examined. With certain cooling rate for a fixed chirality SWNT of (10, 10), the phase change was observed in the temperature range of 200K-220K. For sufficient slow cooling rate, the structure of ice crystal was a hollow octagonal tube. Similar simulations for several host SWNTs with different chiralities such as (8, 8), (9, 9), (11, 11) and (14, 3) were examined. It turned out that for thinner SWNTs the ice crystal favored the hollow tube structure such as pentagonal and hexagonal tubes depending on the diameter. On the other hand, for thicker nanotube the ice tube larger than octagonal structure was not obtained. Depending on the diameter of SWNT, the chiral water tube structure was also observed.