Growth of Single-Walled Carbon Nanotubes from Solid-Phase Cobalt Carbide Nanoparticles by Molecular Dynamics Simulations

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Since single-walled carbon nanotubes (SWCNTs) grow from metal nanoparticles in catalytic chemical vapor deposition (CCVD) process, observation of metal nanoparticles is indispensable for understanding the mechanism of SWCNT growth. While it is difficult to observe nanoparticles in atomic scale experimentally, simulation is useful to observe them.

In this study, we performed molecular dynamics (MD) simulations to investigate the melting point of Co catalyst particle and the time evolution of SWCNT growth, using home-made Tersoff-type and Brenner-Tersoff potential. We put a Co nanoparticle at the center of 10-nm cubic cell and annealed it for 2 ns measuring the kinetic energy and the potential energy of the system, and then supplied carbon atoms into the cell. During the simulation, metal atoms were under Nosé-Hoover thermostat to keep the temperature of the system.

Figure 1 (a) shows the potential energy of pure Co nanoparticles depending on the cluster size and the temperature. We estimated the melting points from the energy jumps and confirmed that the melting point is a linear function of cubic root of the number of metal atoms (Fig. 1 (b)). Though pure Co_{80} and Co_{120} clusters are liquid at 1550 K, they formed solid carbide structure when carbon atoms were supplied to them. The particles remained solid carbide during and after the cap structures appeared (Fig. 2). Carbon atoms adsorbed and diffused on the surface of particles to reach the edge of SWCNTs, and then contributed to the SWCNT growth.

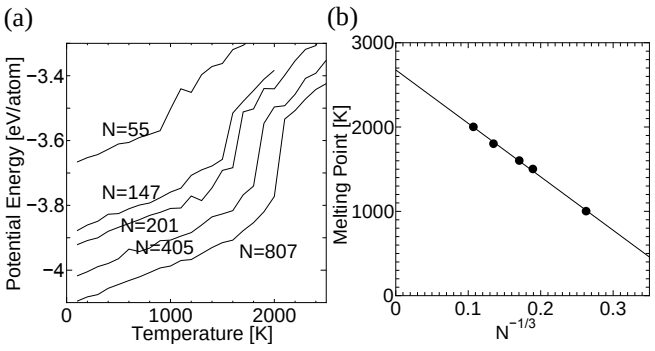

Fig. 1. (a) Energy jump of Co nanoparticles.

(b) Size dependence of melting points estimated from (a).

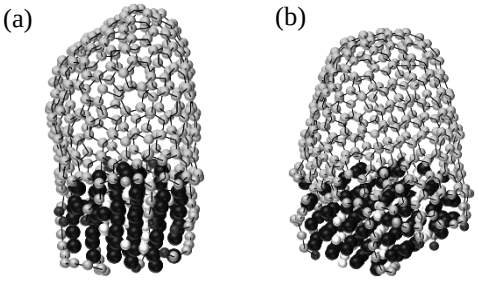

Fig. 2. Co carbide formation and SWCNT growth.

(a) Cubic carbide, 80 Co atoms, 1550 K.

(b) Layered carbide, 120 Co atoms, 1550 K.

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