Molecular Dynamics Simulations of Formation Process of SWNTs in CCVD Method

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Developments of large scale and high-purity generation technique of single-walled carbon nanotubes (SWNTs) are desired for the practical applications of the fascinating new material. In addition to previously known laser-furnace and arc-discharge techniques, recently, the catalytic chemical vapor deposition (CCVD) method has been developed for the possible larger amount production with lower cost. We have developed a high-quality production of SWNTs at low-temperature by using alcohol as carbon source [1]. For the better control of the generation process, understanding of the formation mechanism is inevitable.

We had constructed the classical potential function between carbon clusters and several metal atoms (La, Sc and Ni) based on DFT calculations of small metal-carbon binary clusters for the simulation of the formation process of the endohedral metallofullerene [2]. With the same potential for carbon and Ni, we have explored the formation process of SWNTs in the laser-furnace technique [3]. However, the formation mechanism in CCVD method should be considerably different from the laser-furnace case, because the catalytic metal clusters or particles are present before the assembly of carbon atoms. And carbon atoms should arrive as units of a few atoms determined by the carbon source.

Here, we performed the molecular dynamics simulation of formation process of SWNTs in CCVD method. Starting from randomly distributed carbon atoms and a Ni cluster, the clustering process to a SWNT was simulated. Since the carbon source such as methane and ethanol decomposed to solid carbon only at the catalytic metal surface, the van der Waals potential in the simulation prohibited clustering of carbon-carbon atoms, even though hydrogen or oxygen atoms were not explicitly included. Depending on the initial Ni cluster size and on temperature, the formation of various nanotube cap structures was demonstrated as in examples in Fig. 1.

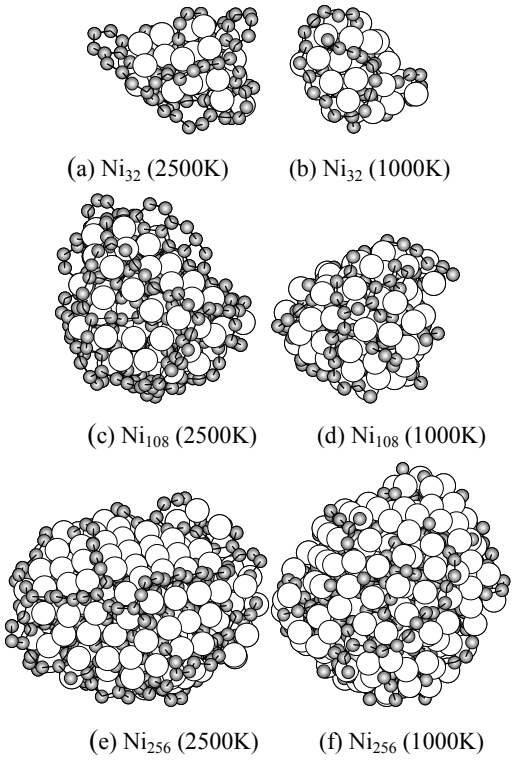

Fig. 1. Aggregation of carbon atoms on Ni particles of various sizes.

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[2] Y. Yamaguchi and S. Maruyama, *Eur. Phys. J. D*, **9**, 385(1999).

[3] Y. Shibuta and S. Maruyama, *Physica B,* (2002), in print.

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