Molecular Dynamics Study of the Role of Transition Metal Atoms in Nucleation Process of SWNTs

○Yasushi Shibuta and Shigeo Maruyama

Department of Mechanical Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

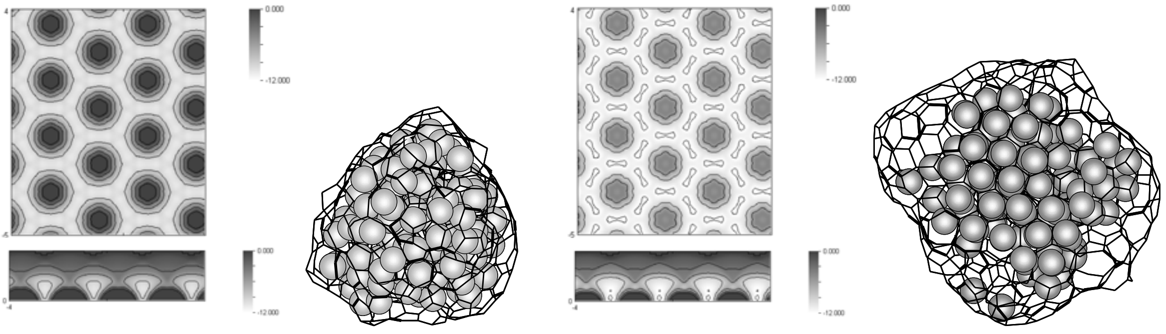
The role of transition metal atoms in the nucleation process of single-walled carbon nanotubes (SWNTs) is studied using classical molecular dynamics (MD) methods and our own potential energy field. We have re-constructed the classical potential function between carbon atoms and several transition metal atoms (Fe, Co and Ni) based on DFT calculations of small metal-carbon binary clusters using Gaussian 98 (B3LYP/LANL2DZ). In these functions, the covalent term is based on a Morse type potential; the parameters are determined by fitting binding energies from DFT calculations to these functions.

In our previous study [1], the clustering process of carbon-containing molecules to transition metal clusters was calculated by MD simulation. The Co cluster was found to have a partially crystal structure where metal atoms are regularly allocated and embedded in a hexagonal carbon network. In the case of Fe, carbon atoms cover the entire surface of the cluster. The number of hexagonal rings in the Co cluster increases about two times faster than in the Fe cluster. This shows the Co cluster has stronger graphitization action than the Fe cluster.

Here, potential energies of M(111) surfaces (M: Fe, Co and Ni) are examined using our original potential functions. Figure 1 shows cross sectional views of the potential energy field at a distance of 1 Å from the (111) surface. Some aspects of the potential differ among metals. Co(111) has the most stable potential field, the shape of which is hexagonal. That may result in the fact that Co cluster was found to have stronger graphitization action in the above-mentioned simulation. Here, we discuss the role of transition metals in the nucleation process of SWNTs using various potential energy surfaces and MD simulation of the clustering process.

[1] Y. Shibuta, S. Maruyama, The 26th Fullerene Nanotubes General Symposium (2004), P. 97.

Corresponding Author: Shigeo Maruyama
Fax: +81-3-5800-6983
E-mail: maruyama@photon.t.u-tokyo.ac.jp



(a) Fe (b) Co

Fig. 1 Cross sectional views of potential energy fileds at 1Å from the (111) surface and snapshots of Fe_{108} and Co_{108} cluster after 100 ns molecular dynamics simulation.