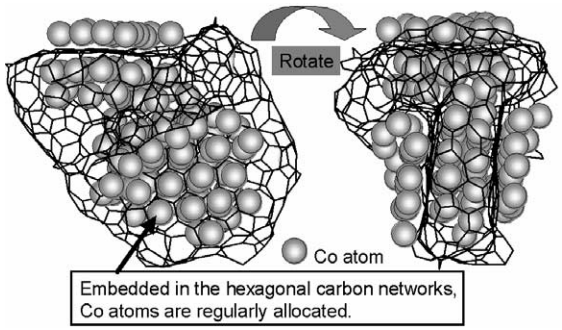
A Molecular Dynamics Simulation of Interaction between Catalytic Metals and Carbon Atoms on Formation Process of an SWNT

○Yasushi Shibuta and Shigeo Maruyama

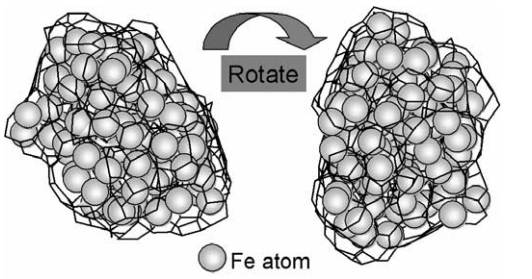
Department of Mechanical Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Interactions between catalytic metals and carbon atoms on formation process of single-walled carbon nanotubes (SWNTs) are studied by molecular dynamics simulations. In our previous study [1], a nanotube cap structure was generated when pieces of the hexagonal network structure extending from inside the cluster merged above the metal surface. Here, we construct 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). These functions have the covalent term based on a Morse type potential; the parameters are determined by fitting binding energies from DFT calculations to these functions. With these potential functions, clustering process of carbon-containing molecules to transition metal clusters (Fe_{108}, Co_{108} and Ni_{108}) are calculated by molecular dynamics method. The simulation technique and initial condition are same as our previous study [1].

Figure 1 shows snapshots after 100 ns. The Co cluster has a partially crystal structure where metal atoms are regularly allocated and embedded in the hexagonal carbon networks (Fig. 1a). This implies a strong interaction between the graphite lattice and the metal atoms. However, there is no allocated part in the Fe cluster. On the other hand, carbon atoms cover the entire surface of the cluster (Fig. 1b). Figure 2 shows a time series of the number of hexagonal rings in these clusters. The number of hexagonal rings in the Co cluster increase about two times faster than in the Fe cluster. This shows the Co cluster has stronger graphitization action than the Fe cluster. It may be deduced that this difference of graphitization action reflects the ability as a catalyst on the formation process of an SWNT.



(a) Co_{108} cluster



(b) Fe_{108} cluster

Fig. 1 Snapshots of the Co and Fe clusters after 100 ns molecular dynamics simulation of the clustering process.

[1] Y. Shibuta, S. Maruyama, Chem. Phys. Lett. 382 (2003) 381.

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

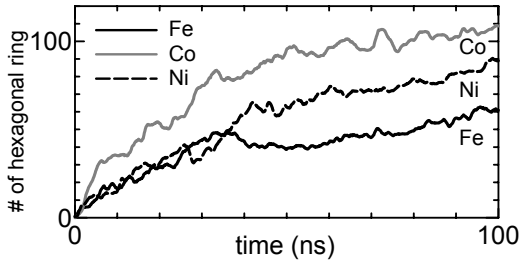


Fig. 2 Time series of the number of hexagonal rings in metal-carbon clusters.