

Nucleation of an SWNT from a catalytic metal cluster inside a carbon nanotube

○Yoshifumi Izu, Junichiro Shiomi and Shigeo Maruyama

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

Molecular encapsulation in the hollow space of a carbon nanotube has attracted interests with various applications. Experiments have been reported on formation of DWNT from C₆₀ fullerenes peapods [1] and ferrocene filled SWNT [2, 3]. The reports demonstrate that the growth mechanism of the inner tube depends on filler precursor.

In this work, we have performed MD simulations of the nucleation process of an SWNT from a catalytic metal cluster inside an SWNT template to gain understanding in the growth mechanism. The same potential models as in the previous work [4] were used. By supplying carbon atoms to a Ni cluster with dissolved carbon atoms placed inside a rigid carbon nanotube, the nucleation process of the inner SWNT was observed (Fig. 1). Simulations were performed for various metal-cluster sizes and outer tube diameters, which resulted in minor differences in the carbon density distribution function of the inner tube (Fig. 2). Additional simulations without van der Waals interaction between inner and outer nanotube resulted in slight decrease of the interlayer distance. The interlayer distances were clearly smaller than the equilibrium distance of carbon atoms. The results suggest that the interlayer distance is determined by the layered distance of metal intercalated graphite.

[1] S. Bandow, et al Phys. Chem. Lett., 337 (2001) 48.

[2] L. Guan, et al., Carbon., 43 (2005) 2780.

[3] H. Shiozawa, et al., Adv. Mater., 20 (2008) 1443.

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

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

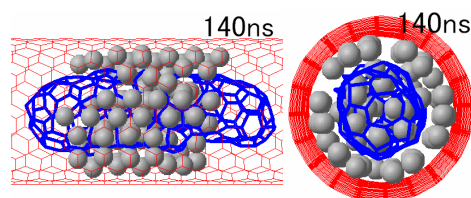


Fig. 1 Nucleation of the inner SWNT from a catalytic metal cluster inside carbon nanotube

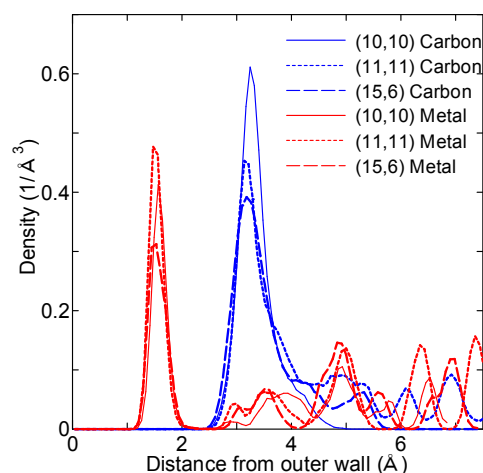


Fig. 2 Density distribution functions of carbon atoms in the inner tube and metal atoms