Nucleation of an SWNT inside a carbon nanotube

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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 C_{60} 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 SWNT nucleation inside an SWNT template based on the potential model as in the previous work [4] to gain understanding in the growth mechanism. The MD simulations were carried out for two cases with different initial conditions and precursor models. In the first case, a Ni cluster with dissolved carbon atoms was initially placed inside the nanotube template, and then the SWNT nucleation was simulated by supplying only carbon atoms (Fig. 1). On the other hand, in the second case, instead of a cluster, Ni and carbon were initially placed inside an SWNT template as individual atoms, and simulations were run by feeding both Ni and carbon atoms with the carbon/metal number ratio of 10, corresponding to that of ferrocene (Fig. 2). As seen in the figures, both cases resulted in the sufficient growth of inner SWNTs. Differences and similarities in growth scenarios, resulting SWNT structures, and growth speeds will be discussed.

[1] S. Bandow *et al.*, *Chem. Phys. 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.

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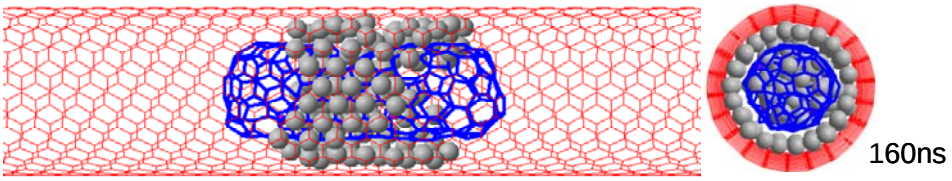

Fig. 1 Nucleation of the inner SWNT from a catalytic metal cluster.

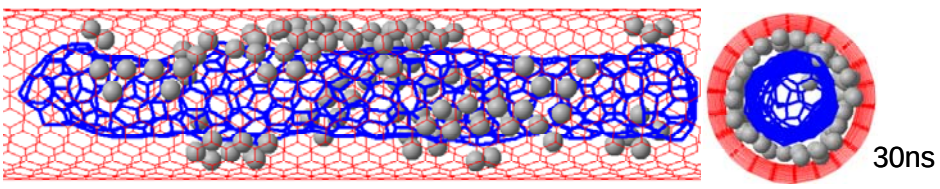

Fig. 2 Nucleation of the inner SWNT from catalytic metal atoms.