Nucleation of an SWNT from a catalytic metal cluster inside a carbon nanotube template: MD simulations of DWNT formation

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Molecular encapsulation in the hollow space of a carbon nanotube has attracted interests with various potential applications. The filling technique has also opened a path to realize controlled chemical reaction in nanoscale chamber for atomic scale selectivity. 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 perform MD simulations of the nucleation process of SWNTs from a catalytic metal cluster inside an SWNT template to gain understanding in the growth mechanism. The methodology is inherited from the previous works on nucleation of SWNTs from isolated catalytic metal clusters [4]. As an initial condition, a Ni cluster with dissolved carbon atoms is placed in a rigid carbon nanotube. By supplying carbon atoms to the metal cluster, with keeping the number of free carbon atoms constant, nucleation of the inner SWNT was observed. Figure 1 shows the nucleation process at different time of the reaction. Once the open surface of the metal cluster is covered with carbon atoms, the feed carbon atoms are adsorbed onto Ni atoms adjacent to the outer-tube wall. Eventually, the supersaturated carbon atoms inside the metal cluster surface lifts of and the cap can be recognized together with the tubal structure. Dependence of the phenomena on the metal-cluster size and outer-tube diameter will be discussed.

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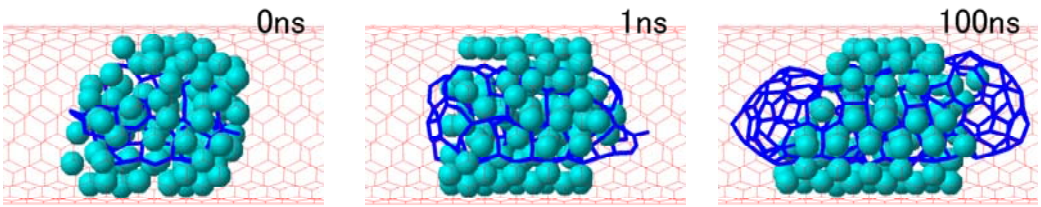

Fig. 1 Nucleation process from a catalytic metal cluster inside carbon nanotube