Molecular Dynamics Simulation of Nanotube Nucleation in Catalytic CVD Method

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The growth process of SWNTs in CCVD method was studied with the classical molecular dynamics simulations. Starting from randomly distributed carbon atoms and a Ni cluster, the clustering process to a SWNT was simulated. In the CCVD process, supported or non-supported catalytic metal clusters are preformed before the assembly of carbon atoms. For the simplicity of the simulation, the floated catalyst condition similar to the floated CCVD process was employed. Assuming that the carbon source molecules such as methane and ethanol decomposed to the solid carbon only at the catalytic metal surface, van der Waals potential prohibited clustering of carbon-carbon atoms, even though hydrogen or oxygen atoms were not explicitly included. Upon arrival of a carbon-containing molecule to the bare metal surface, it was assumed that such reaction would immediately take place. Hence, such reaction barrier was included in the net flux of carbon-containing molecules.

Fig. 1 shows the metal-catalyzed growth of the cap structure on Ni_{108} at 2500K. At the first stage, all carbon atoms attached on the exposed surface and they were absorbed in the metal cluster. When saturated at around 2 ns in this calculation, hexagonal carbon networks were observed inside the metal-carbon binary cluster (a). Some of them precipitated from the surface of the particle, especially the cap structure appeared at the sphere surface of the catalytic metal as if the sphere surface played a roll of the template (b). Continuous supply of the carbon led to the precipitation of hexagonal network from interlayer of crystal (c). After the cap coalesced with the protruding graphitic structure (d), the larger carbon network covered the surface with the certain curvature (e). Furthermore, supersaturated carbon atoms had gradually lifted the surface and the half-cap structure appeared after 40 ns calculation (f). Sequential precipitation from the root lifted up the cap with making the open stem, which can be regarded as the beginning stage of growth process of SWNT (d). In this case, diameter of the cap corresponded to that of metal-carbon binary cluster was about 1.3 nm.

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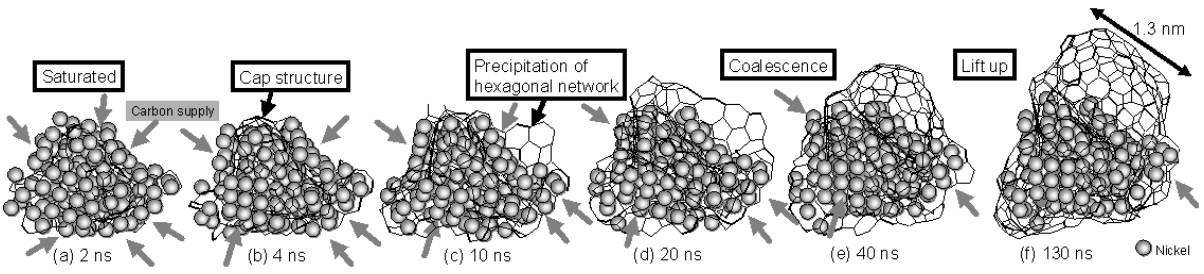

Fig. 1 Snapshots of metal-catalyzed growth process of the cap structure of SWNT.