

Molecular Dynamics Simulation of Nucleation Process of Single-Walled Carbon Nanotubes

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Nucleation process of single-walled carbon nanotubes by the catalytic chemical vapor deposition method is studied by classical molecular dynamics simulation. We start the calculation with randomly distributed carbon-source molecules and a nickel cluster to investigate the metal-catalyzed growth of a cap-structure of a nanotube. When the catalytic cluster reaches saturation with carbon atoms, hexagonal networks are formed both inside and on the surface of the cluster, leading to their precipitation on the cluster's surface and edges. An appropriate nanotube cap structure is generated when pieces of the hexagonal network structure extending from inside the cluster merges above the metal surface. Furthermore, 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. Based on these potentials, interactions between catalytic metals and carbon atoms on formation process of single-walled carbon nanotubes (SWNTs) are also studied.