A Molecular Dynamic Study of SWNT Nucleation and Growth in CVD Method

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In order to explore the possible chirality-controlled growth process, the growth mechanism of single-walled carbon nanotubes (SWNTs) was studied by molecular dynamics simulations. We adopted a newly developed Tersoff-type classical potential for carbon and several metal atoms, such as Co, Ni, Pt, Fe and Ti. We used a genetic algorithm to optimize the potential functions for various solid structures and graphene-metal model predicted by density functional theory.

A metal cluster of certain size and at certain temperature is prepared and is exposed to carbon vapor at certain vapor density (pressure). We can observe the nucleation and growth of SWNTs at certain temperature range and pressure range depending on metal species. In general, higher temperature and lower pressure are preferred for all metal species tested (Co, Fe, Ni, Pt). Higher pressure below the threshold pressure results faster growth simply proportional to the pressure. With the higher pressure beyond the threshold pressure, carbon coating of metal cluster with fullerene-like structure prohibited the growth of SWNTs. Lower temperature than the threshold temperature also results this carbon-coating. Higher temperature simply increased the growth rate with the pseudo-Arrhenius type dependence with an activation energy of about 0.4 eV for Fe. This activation energy is ascribed to the surface or sub-surface diffusion of carbon atoms on a metal cluster.

The threshold temperature is strongly dependent on metal species; much lower for Fe compared to Co. Furthermore, carbon structure interacting to metal cluster during the growth can be classified to two apparently different modes. A preferred structure at lower temperature is “Octopus” mode where several carbon chains are wrapping the metal cluster. Another structure appeared at higher temperature is “Liquid” mode where carbon atoms are dissolved in metal cluster.