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Molecular Dynamics Simulation of Initial Nucleation Process of SWNT from a Metal Particle on a Substrate

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Nucleation process of single-walled carbon nanotubes (SWNTs) from a transition metal cluster on a substrate is studied using classical molecular dynamics (MD) simulations. For describing the effect of the substrate, averaged one-dimensional Lennard-Jones potential is employed between the metal cluster and the bottom boundary of the simulation cell.

Various sizes of the metal cluster are placed on the bottom boundary of the cubic cell. The number of carbon atoms is adjusted to achieve the constant pressure by adding a new carbon atom to the cell when the metal cluster dissolves a carbon atom.

In case of the weak interaction, the metal cluster kept spherical. Some cap structure appeared from the hump of the metal cluster. On the other hand, in case of the strong interaction, metal atoms tend to take (111) crystalline structure parallel to the substrate and graphite network is formed parallel to the direction as if the metal structure works as a template. In this case, graphitic network grows parallel to the substrate and forms the cap structure at this direction. So the direction of the metal (111) structure may be the key of the nucleation of SWNT.

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