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Molecular Dynamics Simulation of Nucleation Process of SWNT from a Metal Particle on a Substrate YASUSHI SHIBUTA, SHIGEO MARUYAMA, Dept. of Mech. Eng., The University of Tokyo — 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. As the initial condition, a Ni500 cluster is placed on the bottom boundary of the cubic cell of 20 nm. The number of carbon atoms is adjusted to achieve the constant density by adding a new carbon atom to the cell when the metal cluster dissolves a carbon atom. As the metal cluster dissolves carbon atoms, the cluster becomes more wetting to the substrate. This may be due to the different wettability between pure metal and metal-carbide. Graphite structure gradually precipitates from the edge of the cluster. Nucleation mechanism of SWNTs will be discussed by comparing with the simulation using the floated catalyst.

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