# Molecular Dynamics Simulations of growth Process of SWNTs in CCVD Method from alcohol

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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. Since the carbon source such as methane and ethanol decomposed to solid carbon only at the catalytic metal surface, the van der Waals potential in the simulation prohibited clustering of carbon-carbon atoms, even though hydrogen or oxygen atoms were not explicitly included. Depending on the initial Ni cluster size and on temperature, the formation of various nanotube cap structures was calculated. In the case of $Ni_{108}$ as a catalytic metal, carbon atoms attached to the exposed surface of catalytic metal and diffused on the surface to make covalent bond with other carbon atoms. Continuous supply of the carbon led to the precipitation of carbon atoms and the growth of the cap structure, which can regard as that of the SWNT. Since almost all carbon was absorbed to the catalytic metal particle after around 100 ns molecular dynamics simulation, we picked up the metal particle with the carbon cap at 100 ns and resupplyed randomly distributed carbon atoms newly in the next calculation. We added 150 and 500 carbon atoms. The density of former was the optimum condition for the growth of cap structure in above calculation, on the other hand that of latter was much higher. Fig. 1 shows snapshots after the 50 ns calculation. The cap structure continued to grow longer in the optimum condition. On the other hand, with higher density the carbon supply rate overwhelm the rate of tube growth and coated all surfaces of metal particle.

In addition, the growth process from alcohol CCVD will be discussed with the simplified algorithm that expresses the purification effect of oxygen radicals.

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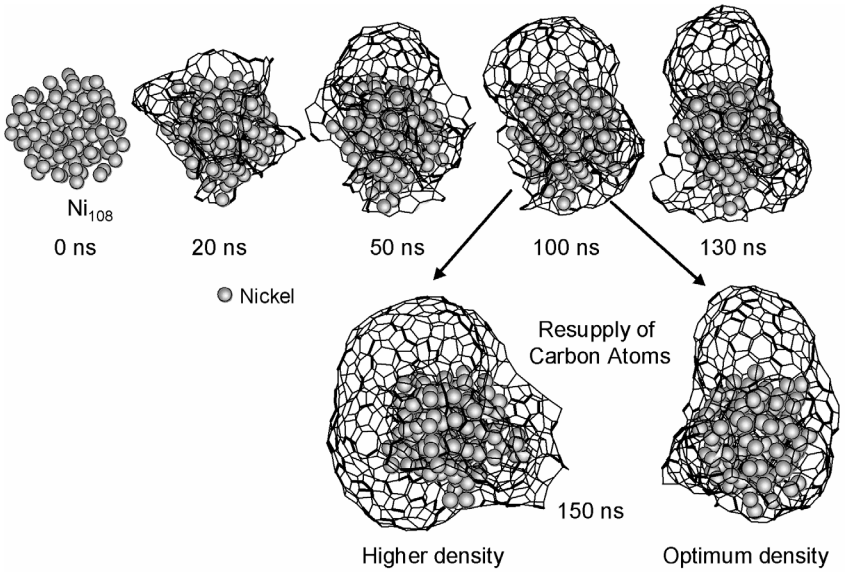


Fig. 1 Snapshots of metal-catalyzed growth process of the cap structure of SWNT.