

Molecular Dynamics Simulations of a Nucleation Process of an SWNT in Alcohol Catalytic CVD Technique

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The nucleation process of a single-walled carbon nanotube (SWNT) considering the dissociation of once-deposited carbon atoms from catalytic metal cluster is studied using classical molecular dynamics (MD) simulations. Experiments suggest that, in the alcohol catalytic CVD (ACCVD) technique, the dissociation of carbon atoms with dangling bonds through the reaction with oxygen atoms may play a key role. As a model system of the ACCVD method, based on the previously reported MD simulation technique [1], the current simulation takes the dissociation process into account. Following an interpretation of the experimental results, the dissociation process is expressed by removing one carbon atom with dangling bonds when three carbon atoms are attached to the metal cluster [2]. Since the dissociation of carbon atoms with dangling bond prevents from the formation of carbon shell around the catalyst cluster, continuous growth after the formation of initial cap structure is expected.

[1] Y. Shibuta, S. Maruyama, Chem. Phys. Lett., 382(2003) 381.

[2] S. Maruyama, Y. Miyauchi, Electronic Properties of Novel Nanostructure (AIP Conf. Proc. 786), 2005, 100-105.