# A Molecular Dynamics Simulation of Generation Process of Nanotubes

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We have performed molecular dynamics simulations of the growth process of metal-carbon binary clusters with the classical potential function [1,2]. As the initial condition, the completely random vapor mixture of 2500 carbon and 25 Ni atoms were allocated in a 585Å cubic fully-periodic simulation cell. Random cage structures of carbon atoms with a few Ni atoms were obtained after 6 ns simulation. Ni atoms on the random cage prohibited the complete closure and anneal of the cage structure into fullerene structure [3].

In the next stage the simulation cell size was artificially shrunk for realization of proceeding collisions of precursor clusters within computational time limit. Fig. 1 shows the growth process of typical tubular cluster from shrinking simulation at 2000K. Even though the structure shown in Fig. 1 is rather ugly, one can see that the tubular structure has grown longer by collisions and coalescences [3].

Separate simulations examined part of the annealing tendency as shown in Fig. 2. An intermediate structure appeared in Fig. 1 (8 ns) was picked up for this annealing with different temperatures (2000K and 2500K). The tubular structure became thick at the narrow part and most straight after 50 ns annealing with both temperature. And, the clustering of Ni atoms was observed for 2500K case.

A completely different initial condition with pre-existing Ni cluster was also tried. An example of the Ni cluster is shown in Fig. 3. Initially almost spherical Ni cluster changed into a sandwiched structure with a graphene sheet in the middle after 500 ps simulation. Several simulations starting from various sizes of initial Ni clusters will be discussed.

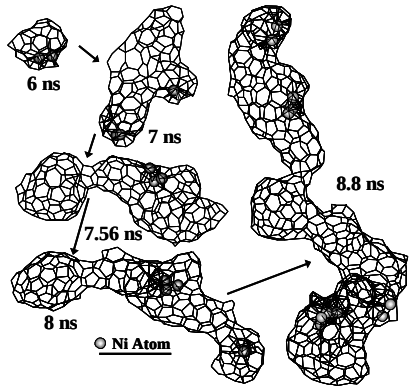


Fig. 1 Growth process of a tubular structure.

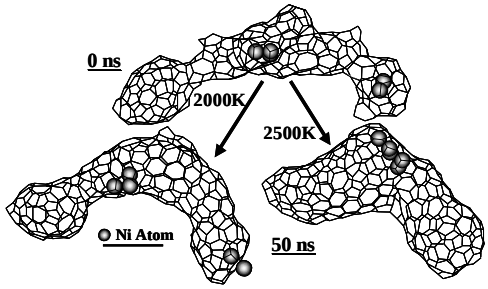


Fig. 2 Annealing of the intermediate structure at 8 ns in Fig. 1.

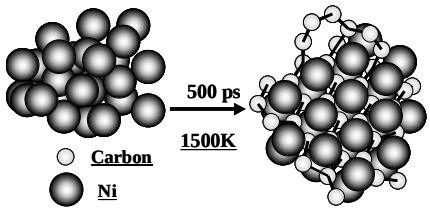


Fig. 3 Snapshots of a Ni cluster in the vapor carbon system.

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