Molecular Dynamics Simulation of Generation Process of SWNTs

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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. Fig. 1 shows a snapshot after 6 ns calculation at 3000K. As shown in the inserted expanded views, many relatively large clusters up to about 100 carbon atoms and a few metal atoms were obtained. Carbon clusters tended to be spherical random cage structure with a few metals on the cage, which prevented from the complete closure of the cage structure.

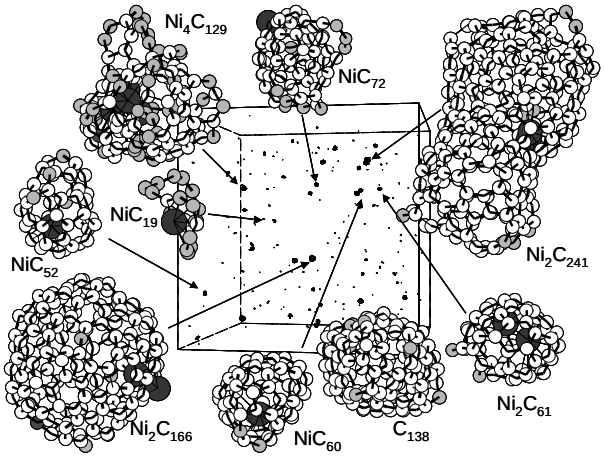

Fig. 1 A snapshot of clustering simulation at 6 ns.

Even though it is expected that the collision rate may be even less at the later stage in the real experimental condition, we slowly shrank the simulation cell to enhance the collisions after 6 ns. The shrinking rate was set as 6×10^{-5}Å per time step or about 12 m/s, which was much slower than the typical translation velocity of clusters. The final structure obtained after 5 ns shrinking simulation at 2000K is shown in Fig. 2. Since most of random cage clusters observed in Fig. 1 were not completely closed they could easily coalesce at the relatively high temperature. Even though the structure shown in Fig. 2 is rather too ugly, the tendency to be elongated network structure is clearly observed. The Ni atoms were slowly assembling to form metal clusters and were trying to find the most stable position, hemi-fullerene cap area. On the other hand, the elongated part tended to be made of pure carbon, and the network structure would be a straight SWNT with metal clusters at each end. The further addition of random cage clusters may be preferentially occurs at these reactive end points.

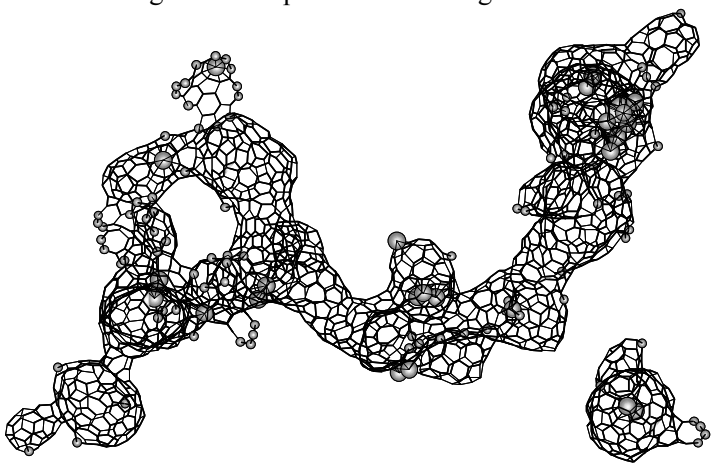

Fig. 2 The structure obtained after collisions of NiC_n clusters.

[1] D. W. Brenner, *Phys. Rev. B*, **42**, 9458(1990).
[2] Y. Yamaguchi and S. Maruyama, *Eur. Phys. J. D*, **9**, 385(1999).

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