Molecular Dynamics Simulation of Precursor Clusters of SWNT Generation

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We have performed molecular dynamics simulations of the clustering process of carbon atoms to investigate the fullerene formation mechanism [1,2], and a new formation model of empty fullerene including the temperature effect was proposed [2]. Further more, based on DFT calculations of various forms of small clusters MC_n and M_n (M = La, Sc, Ni), multi-body classical potential functions for M-C and M-M interactions were constructed with the Morse-type term and the Coulomb term as functions of coordinate number of a metal atom [3]. With that potential function, we have studied in detail the difference of the growth processes among La or Ni containing systems and those of carbon only to investigate the effect of metal atoms. In this report, we compared mass spectra of clusters in the case of the simulation with C and Ni atoms.

The potential functions were the same as our previous reports [1-3]. The clustering process starting from randomly distributed 2500 carbon and 25 Ni atoms in a 585Å cubic cell were simulated under the controlled temperature condition, where the translational, rotational and vibrational temperatures of cluster were kept nearly equilibrium at T_C = 3000 K.

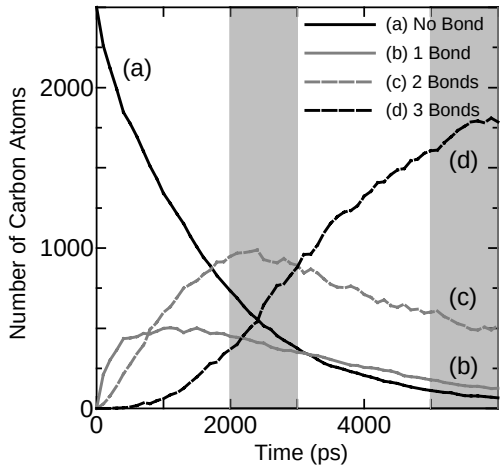

Fig. 1. Time change of number of carbon atoms with specific coordination number.

Carbon atoms were classified into 4 groups according to its coordination number, number of bonds. Fig. 1 shows the time change of number of carbon atoms with each coordination number. At first, the carbon atoms with dangling bonds increase while isolated atoms decreased. The number of atoms with no dangling bonds became dominant at 3000 ps. At 6000 ps, most of carbon atoms had no dangling bonds and the structure was random-cage with Ni atoms preventing the full closure.

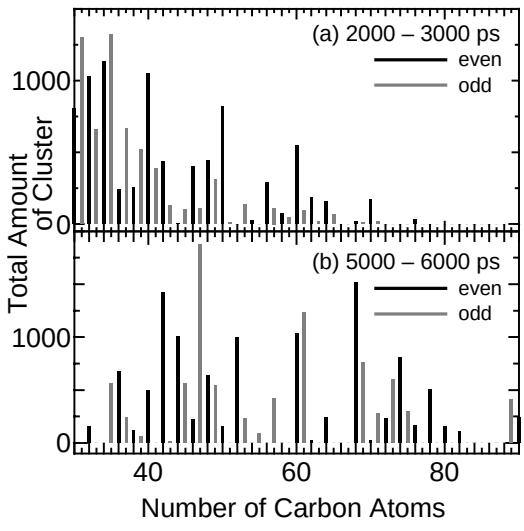

Fig. 2. Histgram of clusters

Fig. 2 shows the cumulative number of clusters between 2000 – 3000 ps and between 5000 – 6000 ps. The clusters with even number of carbon atoms were observed much than those with odd number for clusters larger than 40 atoms. This tendency is in good accordance with FT-ICR cluster beam experiments [4].

References

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3. Y. Yamaguchi and S. Maruyama, *Eur. Phys. J. D*, **9**, 385(1999).
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