A Molecular Dynamics Simulation of Metal-Containing Fullerene Formation

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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, the formation process of metallofullerene was studied using the similar molecular dynamics simulations [3]. 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]. In this report, the difference of the growth processes among La or Ni containing systems and those of carbon only were studied to investigate the effect of metal atoms.

The potential functions were the same as our previous reports [1-3]. The clustering process starting from randomly distributed 2500 carbon and 25 metal 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 shows the cumulative number of clusters between 2900–3000 ps per 10 ps. When La or Ni atoms were applied as the additional metal, clusters with 30-70 carbon atoms and with a metal atom appeared, as in Fig. 1(b)(c). However, few cluster of the same size range was observed for pure carbon system in Fig. 1(a). The promotion of quick growth of large cluster with La or Ni atoms is in good accordance with FT-ICR cluster beam experiments [4].

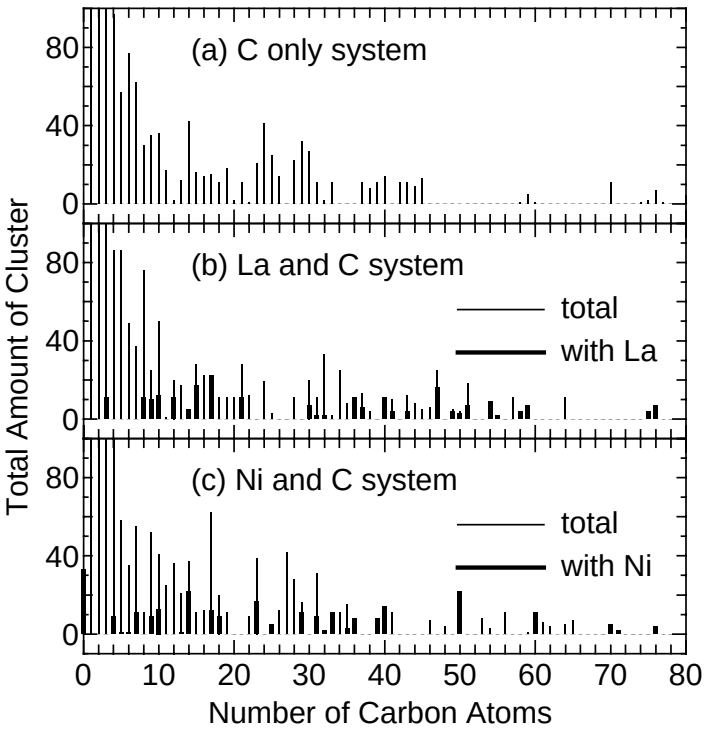

Fig. 1. Cumulative number of clusters between 2900-3000 ps (per 10 ps).

References

1. Y. Yamaguchi and S. Maruyama, *Chem. Phys. Lett.* **286**, 336(1998).
2. S. Maruyama and Y. Yamaguchi, *Chem. Phys. Lett.* **286**, 343(1998).
3. Y. Yamaguchi and S. Maruyama, *Eur. Phys. J. D*, **9**, 385(1999).
4. S. Maruyama *et al*., *Fullerene Sci. Tech.*, **7**, 621(1999).