La, Sc 内包フラーレン生成の分子シミュレーション

Molecular Simulations of the Formation of La, Sc Containing Fullerene

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The growth process of metal-containing fullerenes is studied by using the molecular dynamics method which is similar to our simulations of prefect C_{60} and C_{70} formation[1,2]. In order to model the potential function between carbon and metal atoms appropriate for the MD simulation, the binding energy and charge state of various forms of small clusters MC_n (M = Sc, La, Ni) were calculated with the density functional theory based on the Becke's three-parameter exchange functional with the Lee-Yang-Parr correlation (B3LYP). A multi-body potential function was constructed as a function of coordinate number of a metal atom. Here, the Coulomb term and the Morse-type term were separately described considering the large charge transfer from a metal atom to carbon atoms.

The clustering process starting from 500 isolated carbon atoms and 5 scandium atoms in a 342 Å cubic cell was simulated under the controlled temperature condition, where the translational, rotational and vibrational temperatures of each cluster were kept nearly equilibrium at T_c = 3000 K. Fig. 1 shows the growth process of a $Sc@C_{92}$ cluster obtained at 3000 ps. The vertical position and horizontal length denote the size and the duration of existence of clusters, respectively. When the cluster was smaller than $Sc+C_6$, a fan-type structure was reproduced around the scandium atom. When it grew to about $Sc+C_8$, the scandium atom positioned out of the monocyclic carbon ring. Then, the scandium atom approached to the center of the monocyclic ring when the cluster grew as large as $Sc+C_{13}$. The host monocyclic ring changed to a bi-cyclic ring with keeping the scandium atom in the same plane around C_{16}. When the host carbon cluster grew as large as C_{19}, it annealed to a graphitic sheet and the scandium atom was driven out of the plane. Here, the Coulomb force induced curvature to the sheet, and the cluster grew larger until about $Sc+C_{27}$ keeping the open-cap structure. Then, in this case, a collision with a large cluster of C_{38} prevented gradual growth and resulted in the formation of $Sc@C_{66}$ where the scandium atom was almost enclosed in the carbon cage. The number of carbon atoms was not enough to form a complete closed cage until around C_{84}, when a hollow caged structure similar to fullerene cage first appeared. Considering the difference of time and temperature scale between the real phenomena and simulation, these hollow caged structures could have sufficient collision free annealing interval to form more sophisticated structures like experimentally isolated metal-containing fullerenes. By comparing three metal atoms of Sc, La and Ni, we will consider the the possibility of encapsulation or the difference of the encapsulation characteristics such as number of metal and carbon atoms and structures of carbon cage.

References: (1) Y. Yamaguchi & S. Maruyama, Chem. Phys. Lett. **286**, 336 (1998). (2) S. Maruyama & Y. Yamaguchi, Chem. Phys. Lett. **286**, 343 (1998).

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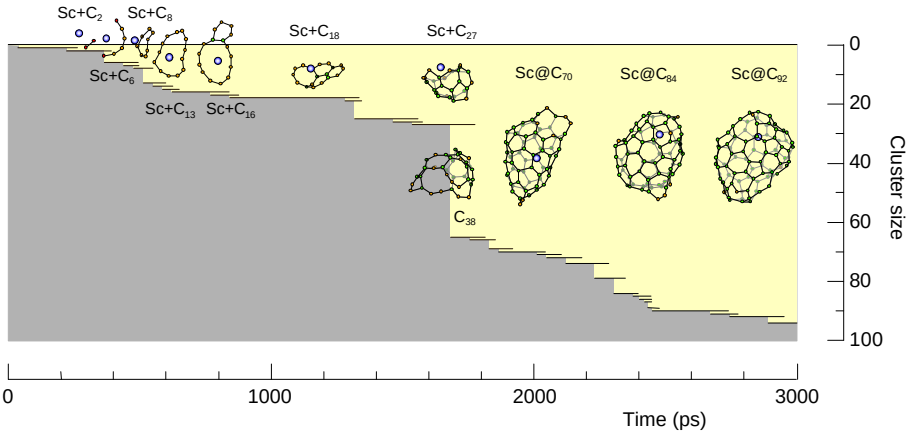

Fig. 1　Growth process of a scandium-containing fullerene.