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Molecular Dynamics of the Formation Process of Fullerene

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The formation mechanism of fullerene, a new type of carbon molecule with hollow caged structure, was studied using the molecular dynamics method. The classical potential developed by Brenner[(1)] was employed with the simplification. The clustering process starting from isolated carbon atoms was simulated under the constant internal temperature control[(2)]. Considering that the time scale of the simulation was compressed, the equilibrium of internal and translational temperature was artificially enforced.

Typical result of the simulation is shown in Fig. 1. Here, 550 carbon atoms were located at random positions with the random velocity as the initial condition. Then, the total translational energy and total internal energy of each cluster were kept at 3000 K. Until 25 ps, there were only small chains up to about C_{10}. At 60 ps there appeared some multi-cyclic rings of about C_{20}. Then, at 125 ps, three dimensional pieces were formed. Finally at 200 ps there was a large fullerene like caged structure and some flat graphitic structures.

The effect of the temperature on the finally obtained structure is complied in Fig. 2. The structures of obtained clusters depended on the control temperature, yielding to graphitic sheet for T < 2500, fullerene-like caged structure for 2500 < T < 3500, and chaotic 3-dimensional structure for T > 3500. The clustering process leading to the caged structure in contrast to the flat graphitic structure was studied in detail. In the clustering process yielding to the caged structure, the moderate sized precursors with large vibrational energy transformed to the random 3-dimensional structure. On the other hand, in the clustering process yielding to the flat structure, the precursors with the lower vibrational energy always kept the graphitic structure.

The possibility of obtaining considerable amount of C_{60} will be discussed.

References

(1) Brenner, D. W., Phys. Rev. B, 42-15, (1990), 9458. (2)Maruyama, S. and Yamaguchi, Y.: Thermal Sci. & Engng., 3 (1995), 105.

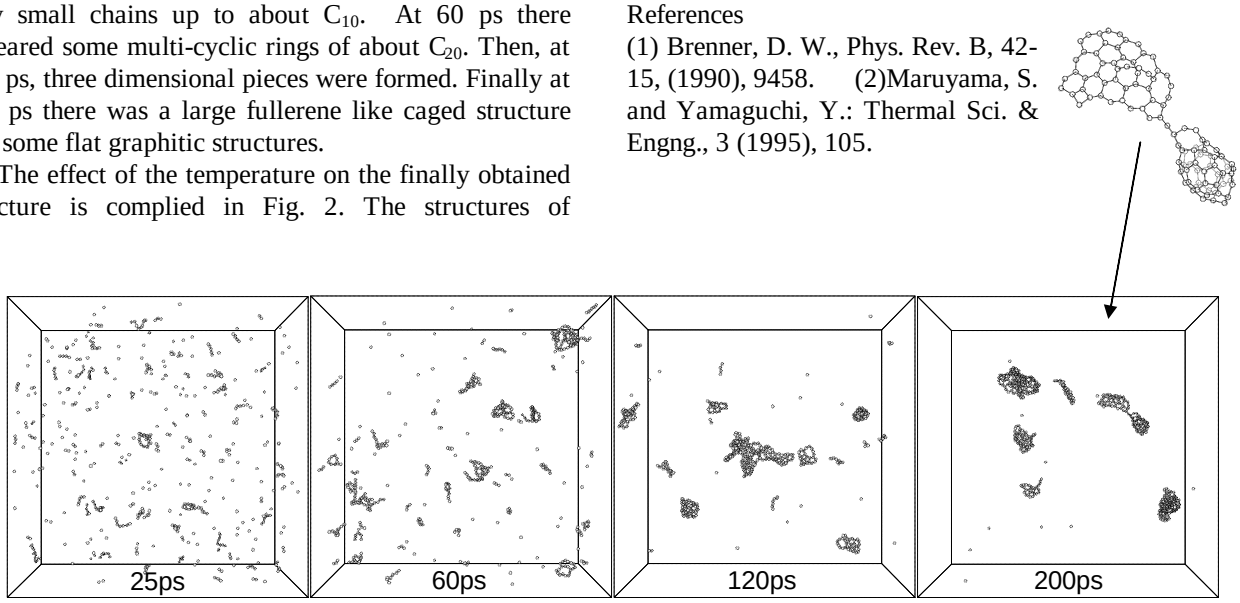

Fig. 1 Assembly of fullerene structure from randomly distributed 550 carbon atoms at 3000K

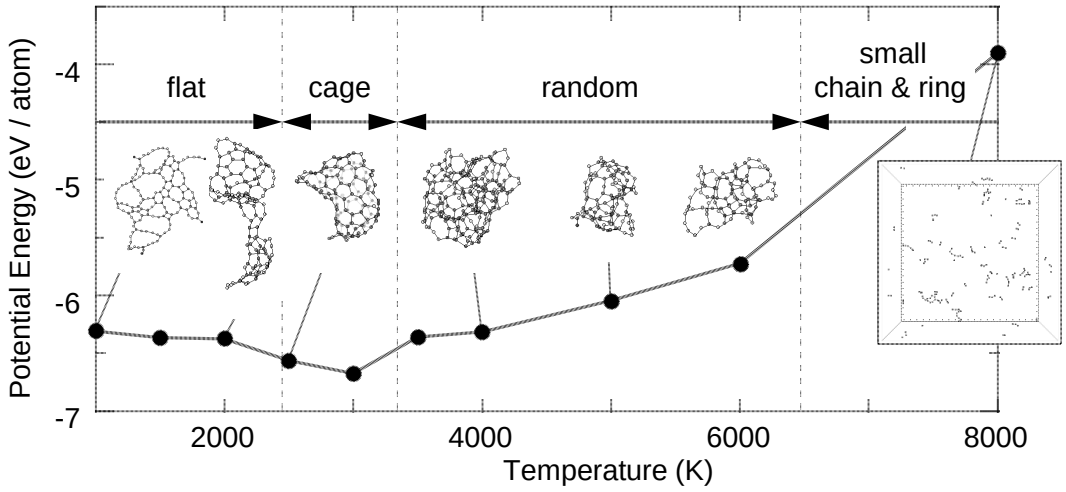

Fig. 2 Structures of clusters at various temperature