Atomic density dependence of formation of polycyclic aromatic hydrocarbon by molecular dynamics simulation

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We have been studying the formation and deformation processes of nano-carbon molecules by use of molecular dynamics (MD) simulation. We deal here with the formation of hydrocarbon dust in the interstellar space. The purpose of this study is to make clear the growth of hydrocarbon dust from carbon atoms, hydrogen atoms and their small molecules.

In the MD simulation, the carbon and hydrogen atoms were initially located at random in a simulation box under periodic boundary condition. Chemical interaction between atoms was represented by the modified Brenner reactive empirical bond order potential [1] and temperature was controlled by the Langevin thermostat regarded as background radiation.

As a simulation result, polycyclic aromatic hydrocarbons (PAH) occurred and the following formation process was clarified. First, many carbon chain molecules occurred. Next, long carbon chains made carbon rings with tentacle, which is called “octopus structure”. Finally, the rings and tentacle were knitted into six-membered rings and then they were formed into the PAH like a graphene. In addition, amorphous carbon did not appear.

This MD simulation treated high atomic density and short time scale. However, under the assumption that the collision number of molecules is in proportion to atomic density, this formation process of PAH corresponds to a phenomenon for 300 year on the atomic density of 100 atom/cc. The second point that requires clarification is whether this assumption is valid. To clarify its point, we execute the MD simulations on deferent atomic densities and we compare formation speeds.

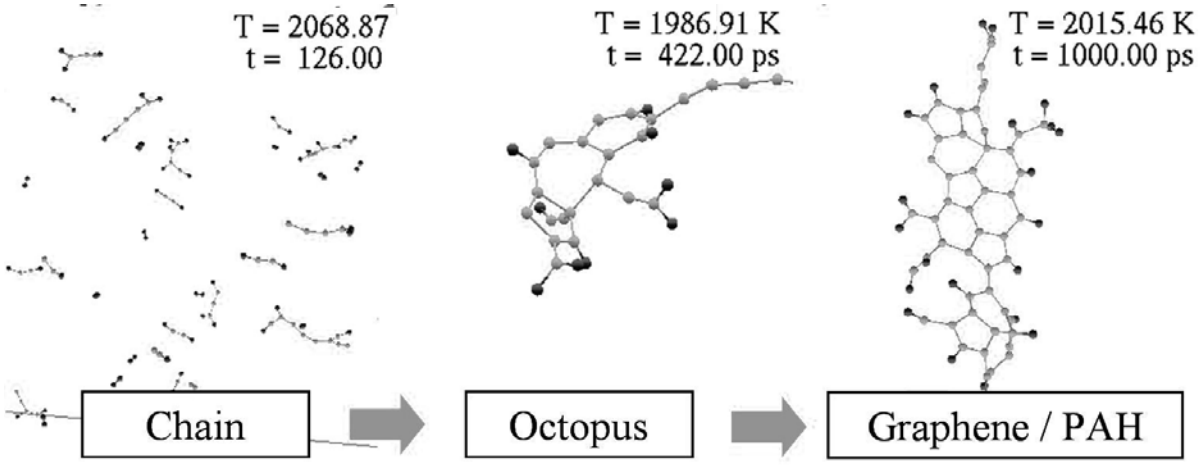

Figure 1: Formation process. The gray and black spheres indicate carbon and hydrogen atoms, respectively.

References

[1] A. Ito and H. Nakamura, Commun. Comput. Phys 4 (2008), 3, 592.