§4. Ab initio Molecular Dynamics Study of Graphite Erosion and Formation of Hydrocarbon Molecules: Absorption of Many Hydrogen Atoms and Behavior at High-temperature Region

Koga, T. (AA&S Co., Ltd.), Tanaka, M.

The most important and urgent thing for achievement of magnetically confined nuclear fusion may be to find suitable wall materials of a fusion reactor having both heat and radiation resistances. Researches show that the wall surface is damaged not only by the physical sputtering process but also through chemical reactions (sputtering), the latter of which is confirmed to have major influences on the damaging of the fusion reactor wall.

As a typical example of the chemical sputtering, we study the erosion process of graphite by means of the *ab initio* (first-principle) molecular dynamics (MD) simulation code SIESTA [1]. In the code, the electron distributions in materials are determined by solving the Kohn-Sham equation, which is based on the density functional theory of quantum mechanics. We use parallel computers (PC Cluster) each consisting of four Pentium 4/64-bits to handle massive computations [2].

Previously we found by *ab initio* MD simulation that hydrocarbon molecules CH_n with n>1 are not formed on a flat (undamaged) graphite because of strong attraction between H and C atoms [3]. Experimentally, on the other hand, hydrocarbon molecules are generated through the chemical sputtering when graphite absorbs large number of hydrogen atoms. Being enlightened by this experiment, we have started a new series of *ab initio* MD simulations.

We used the simulation system made of five carbon layers of graphen sheets [4], and found that the graphite layer is deformed to a highly non-flat shape (hills and valleys) and that hydrocarbon molecules are formed when the number of adsorbed hydrogen atoms per graphite layer reaches about 50%. Moreover, we studied the behavior of hydrocarbons at high temperature region using MD with the Nose thermostat. As shown in Figure 1, a CH_3 molecule already formed at low temperatures is detached from the graphite layers at high temperature 900K.

From these results, we conclude that chemical sputtering is operative at low temperatures and that already formed hydrocarbon molecules are detached at high temperatures. Thus, we propose to control the plasma not to penetrate deeply into the material such that less chemical sputtering takes place. It may be possible that the material ablation by chemical sputtering is reduced by keeping carbon materials at high temperatures (about 1000K) because hydrocarbon molecules are not easily generated at high temperatures.

In conclusion, we qualitatively established the mechanism of the chemical sputtering by using the quantum-mechanics based computer simulation. In the near future, quantitative research is required not only for through understandings of the phenomenon but also for material development of fusion device walls.

References

[1] SIESTA (Spanish initiative for electronic simulations with thousands of atoms): at http://www.uam.es/departamentos/ciencias/fismateriac/siesta/
[2] M. Tanaka, Los Alamos Archive, physics/ 0407152 (2004)
[3] Y.Zempo and M.Tanaka, Newsletter of National Institute for Fusion Science (February, 2004).
[4] T. Koga and M. Tanaka, J. Korean Phys. Soc., vol.49, S52-55 (2006).

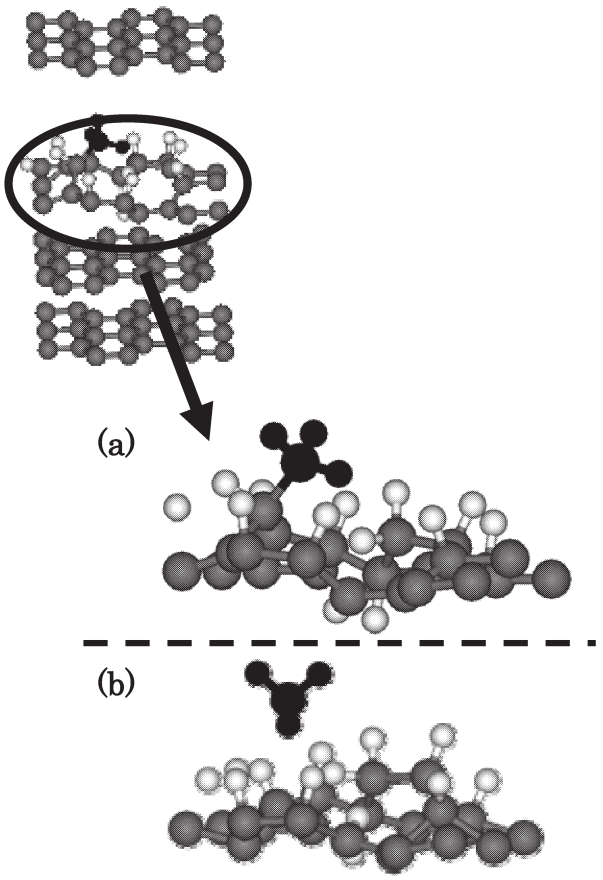

Fig. 1. Formation of CH_3 molecule on the graphite layer by Nose thermostat MD at 900K. (a) at time 0 fs、(b) at time 42.6 fs. Gray balls are carbon atoms, white balls are hydrogen atoms, black balls are CH_3 molecule.