# §30. Energy Flow during Hydrogen Atom Adsorption on a Graphite Surface by Molecular Dynamics and VR Visualization

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We have investigated chemical sputtering on plasma facing materials of divertor walls composed of graphite by the use of molecular dynamics simulation [1]. Processes of chemical sputtering depend on the structures of graphite materials [2]. However, they have the following scenario in common. In chemical sputtering, unstable atom of surfaces can cut a covalent bond by using kinetic energy which is raised by incidence of hydrogen atom, and then $H_2$ and hydrocarbon molecules are detached from surfaces. Here, importance is that not only the incident energy of hydrogen atom but also adsorption energy, which is difference of energies between the state where hydrogen atom is bound by a surface and the state where hydrogen atom is far from the surface, are converted into the kinetic energy of the atom of surfaces. From this reason, to follow the collision of atoms only is not enough to understand the chemical sputtering. If we can know energy flow during interaction between hydrogen and carbon atoms, it is helpful to clarify the mechanism of chemical sputtering. In this paper, we create new theory to formulate energy current between atoms for multi-body potential well used by molecular dynamics [3]. Moreover, this energy current is visualized in 3-dimentional virtual reality space by using our original software AI-Score with CAVE system [4].

In this theory, to derive energy flux between atoms due to interaction, the field of energy density $e(\vec{x},t)$ in the classical particle system is defined by

$$e(\vec{x},t)=\sum_i\left[\frac{\vec{p}_i{}^2(t)}{2m_i}+u_i(t)\right]\delta(\vec{x}-\vec{r}_i(t)),$$

where $\vec{x}$ is coordinates of space, $m_i$, $\vec{r}_i$ and $\vec{p}_i$ are mass, position and momentum of particle, respectively. The interaction energy of particle $u_i(t)$ satisfies $U(r)=\sum_i u_i(t)$ with total interaction energy $U(r)$. Here, we can consider energy flux field satisfying the continuity equation given by

$$\frac{\partial e(\vec{x},t)}{\partial t}+\nabla\cdot\vec{j}(\vec{x},t)=0\cdot$$

In this theory, the energy flux field is consists of two terms. One is the energy flow due to the movement of particles, and the other is the energy current between particles due to interaction. Consequently, in the latter term, the energy current from the $i$ th particle to the $k$ th one is obtained by

$$\vec{j}^{\,\mu}_{ik}=\frac{1}{2}\left(\frac{\vec{p}_i(t)}{m_i}+\frac{\vec{p}_k(t)}{m_k}\right)\cdot\frac{\partial U(r)}{\partial\vec{r}_{ik}},$$

where $\vec{r}_{ik}=\vec{r}_i-\vec{r}_k$. This energy current between particles is calculated by molecular dynamics simulation easily. From Fig 1., it is understand that a graphene surface obtained energy about 2 eV due to hydrogen atom adsorption. VR visualization by AI-Score with CAVE enables us to directly watch the energy flow in the complicate molecular and crystal structures, in which magnitude of energy current is shown by color and the direction of it is shown by allow (Fig. 2). In future, mechanism of chemical sputtering on graphite will be clarified by using the theory of energy flow and VR system.

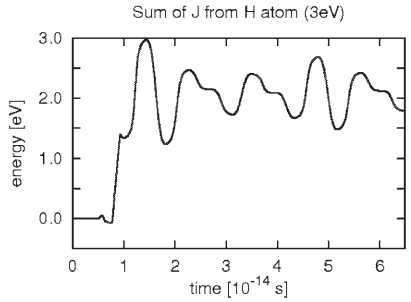


Fig. 1: Time integration of energy current from adsorbed hydrogen atom into a graphene surface.

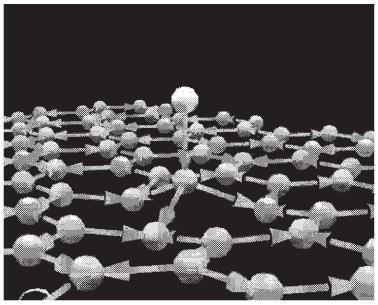

Fig. 2: Visualization of energy current between particles during hydrogen atom adsorption.

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[4] Cruz-Neira, C. et al: ACM SIGGRAPH 93 (1988) 65.