# §25. Dynamics of Hydrogen Atom Injected into Graphite Using Molecular Dynamics Simulation

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Divertor wall experiences plasma bombardment in magnetic confinement nuclear fusion device. Especially, hydrogen plasma is absorbed by the graphite of the divertor because a hydrogen atom prefers to create a covalent bond with a carbon atom. The graphite absorbing hydrogen atoms becomes weak and then it is easy eroded. Absorbed hydrogen atoms cause chemical sputtering and yield hydrocarbon molecules. The hydrocarbons obstruct plasma confinement. The erosion of graphite and the generation of hydrocarbon molecules should be restricted. We therefore have investigated interaction between hydrogen atom and graphite in atomic scale using molecular dynamics simulation. In the present paper, the dynamics of hydrogen atom injected into a graphite (0 0 0 1) surface at the incident energy of less than 30 eV is reported [1].

The single crystal graphite, which consists of graphene sheets stacking at the distance of 3.35 Å, was maintained by interlayer intermolecular forces. We prepared eight graphene sheets measuring $2.00 \times 2.17$ nm$^2$ and a simulation box having same sizes in the x and y directions with periodic boundary condition. Hydrogen atoms were injected into the graphite (0 0 0 1) surface perpendicularly. This system includes two kinds of interactions. One is chemical interaction creating covalent bonds which is represented by modified Brenner reactive empirical bond order potential model and intermolecular interaction giving interlayer force which is represented by our new potential model. The time is developed using symplectic integration with the time step of $5 \times 10^{-18}$ s.

The dynamics of hydrogen atom in the graphite at the three cases of the incident energy of 5 eV, 15 eV and 30 eV are treated. When the incident energies were 5eV, almost all hydrogen atoms were adsorbed on the front surface of the first graphene layer, where the graphene layers are here numbered from surface side. In the case of the incident energy of 15 eV, the graphite hardly adsorbed hydrogen atoms and then almost all hydrogen atoms were reflected by the first graphene layer. In the case of the incident energy of 30 eV, hydrogen atoms penetrated the first graphene, bounded between the first and second graphene layers and adsorbed by the back surface of the first graphene or the front surface of the second graphene. Namely, hydrogen intercalation occurred. Thus, the dynamics of hydrogen atom in graphite depended on the incident energy.

Our previous simulation in which the potential model of interlayer interaction is not used did not demonstrate the hydrogen intercalation because the layer structure of graphite had changed into an amorphous structure rapidly. Therefore, the interlayer interaction supporting graphene layers plays an important role in the hydrogen intercalation on the graphite. The dependence of the dynamics of hydrogen atom on the incident energy is explained by the simulation result in the research of reaction between a single hydrogen atom and a single graphene. The reaction between a single hydrogen atom and a single graphene are classified into adsorption, reflection and penetration and then adsorption, reflection and penetration rates have peaks at the incident energy of 5 eV, 15 eV and 30 eV, respectively. The dynamics of hydrogen atom in the graphite, which is layered graphene, can be regarded as the succession of the reaction between a single hydrogen atom and a single graphene. The adsorption at the incident energy of 5 eV and the reflection at the incident energy of 15 eV on the front surface of the first graphene layer agree with adsorption and reflection between a single hydrogen atom and a single graphene. As the incident energy decreases from 30 eV, dominant reaction between a single hydrogen atom and a single graphene shifts in order of penetration, reflection and adsorption. In this manner, the hydrogen atom intercalated by graphite in the case of the incident energy of 30 eV experienced penetration, reflection and adsorption to reduces its kinetic energy due to interaction with each graphene layer. After the hydrogen atom penetrates the first graphene layer, it repeats reflection between layers and then it is adsorbed by the first or second graphene. Thus, the dynamics of hydrogen atom in graphite depends on the incident energy, and its mechanisms are explained by the reaction with a single graphene.

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[1] A. Ito and H. Nakamura, Commun. Comput. Phys. 4 (2008) 592.
[2] H Nakamura, A. Takayama, A. Ito, Contrib. Plasma Phys. 48 (2008) 265.