§27. Molecular Dynamics Simulation of Hydrogen Injection on Diamond Surfaces

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We have been developing [1,2,3,4,5] molecular dynamics (MD) simulation of interaction between hydrogen and graphite using a modified Brenner empirical bond order potential(REBO) model [3,6,7]. In our previous studies where hydrogen injection onto the surface of either graphene or graphite was treated, we obtained qualitatively the injection energy dependence of the hydrogen adsorption ratio due to graphene or graphite. Moreover, the dynamics of adsorption process was also revealed by observing the motion of hydrogen and carbon atoms. Thus, we showed that our MD simulation using the modified REBO potential is a powerful tool, useful in the determination of the reaction process in the atomic level.

In this work, we report hydrogen injection onto the surface of diamond, which is also composed of carbon like graphene and graphite. The main difference between diamond and the others (i.e., graphene and graphite) is a crystal structure. The carbons of diamond are linked by a sp^3 covalent bond. On the other hand, the bonds between the carbons of graphene and the intralayer bond in each layer of graphite are sp^2 covalent bonds. In the modified REBO potential, the sp^3 covalent bond between carbons can be treated as well as the sp^2 bond. We, therefore, simulate hydrogen injection onto the diamond by our MD simulation code.

As the initial simulation model, the carbon atoms are set as the lattice point which composes the diamond crystal structure. We choose ***a, b*** and ***c*** axes of the diamond crystal as ***x, y*** and ***z***-coordinates, respectively. The periodic boundary condition is applied to ***x*** and the ***y*** directions. Hydrogen atoms are injected onto the diamond surface which is identified by (001). The injection angle of hydrogen is perpendicular to the surface.

As the simulation result, it was found that, when the kinetic energy of the injected hydrogen is less than 0.3 eV, the temperature of the diamond is saturated without increasing, even though the hydrogen atoms are being kept injecting to the diamond. When the kinetic energy is larger than 0.3 eV, the temperature is increased and the diamond structure is eroded gradually. From the observation of the motion of the atoms, the saturation of the temperature in the case that kinetic energy of the hydrogen is less than 0.3 eV is caused by the adsorption of hydrogen on the diamond surface. It is summarized that, once the adsorbed hydrogen coats the diamond surface, the coating hydrogen prevents other hydrogen from interacting directly with carbon atoms. This hydrogen coating operates when the hydrogen energy is less than 0.3 eV, and it is destroyed by the hydrogen whose kinetic energy is more than 0.3 eV.

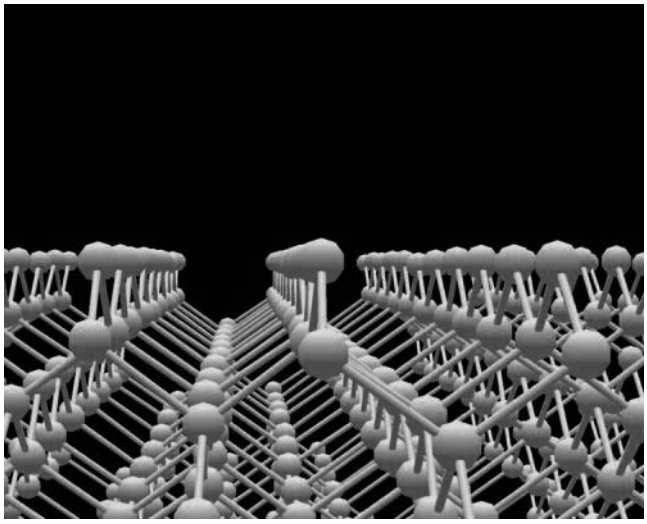

Fig. 1. Snapshot of diamond surface (100). We impact hydrogen atoms from the top of the surface.

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