Dependence of saturation temperature on diamond surfaces adsorbing hydrogen

H. Nakamura[a,b], A. Ito[a], S. Saito[b], Y. Tamura[c], S. Fujiwara[d], N. Ohno[b], S. Kajita[e]

[a]*National Institute for Fusion Science,322-6 Oroshi-cho, Toki 509-5292, Japan*
[b]*Department of Energy Engineering and Science, Graduate School of Engineering, Nagoya University, Nagoya 464-8603, Japan*
[c]*Konan University, 8-9-1 Okamoto, Higashinada-ku, Kobe 658-8501, Japan*
[d]*Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*
[e]*EcoTopia Science Institute, Nagoya University, Nagoya 464-8603, Japan*

hnakamura@nifs.ac.jp

We have been developing [1-5] 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.

In this paper, we report hydrogen injection onto the surface of diamond, which is also composed of carbon like 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 ***y*** directions. Hydrogen atoms are injected onto four types of the diamond surface, which are identified by (100), (110), (111) and (120), respectively.

As the simulation result, it was found that, when the kinetic energy of the injected hydrogen is less than 0.3eV, the temperature of the diamond is saturated without increasing, even though the hydrogen atoms is continued to inject to the diamond. We also found that the saturation temperature depends on the surfaces of diamond. This dependence is caused by the difference of the most stable binding energy between a hydrogen atom and each surface of diamond. Estimating the saturation temperature by the biding energy and the surface coverage which are given by the simulation, we showed that our estimated saturation temperatures almost agree with the simulation results.

[1] A. Ito and H. Nakamura, J. Plasma Phys., **72** (2006) 805.
[2] A. Ito and H. Nakamura, Thin Solid Films, **516**, (2008) 6553.
[3] A. Ito and H. Nakamura, Commun. Comput. Phys., **4** (2008) 592.
[4] A. Ito and H. Nakamura, Jpn. J. Appl. Phys., **47** (2008) 4715.
[5] A. Ito and H. Nakamura, and A. Takayama, J. Phys. Soc. Jpn., **77**(2008) 114602.
[6] D. W. Brenner, Phys. Rev. B **42** (1990) 9458 [Errata; **46** (1992) 1948].
[7] D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni and S. B. Sinnott, J. Phys., Condens. Matter, **14** (2002) 783.