§29. Molecular Dynamics Simulation of Sputtering Process of Hydrogen and Graphene Sheets

Nakamura, H.,
Takayama, A.,
Ito, A. (Nagoya Univ.)

To clarify the yielding mechanism of small hydrocarbon molecules in chemical sputtering between hydrogen and graphene sheets[1, 2, 3, 4], we made classical molecular dynamics simulation with modified Brenner's REBO potential which we proposed to deal with chemical reaction[5, 6, 7, 8, 9].

As the simulation model, we prepared[9] more realistic physical system, which is composed of 160 incident hydrogen atoms and ten graphene multilayers (Fig.1), than our previous model[7].

We calculated the radial distribution functions $g(r)$ among carbon atoms in the third graphene sheets numerically, as shown in Fig.2. From the present work[9], we found the following fact: breaking the covalent bonds between carbon atoms by hydrogen does not play an important role during destruction process of graphene structure, but momentum transfer from incident hydrogen to graphene causes to destroy graphene structure. Moreover, it is found[9] that almost all fragments of graphene sheets form chain-shaped molecules, and that yielded hydrocarbon molecules are composed of carbon chain and single hydrogen-atom.

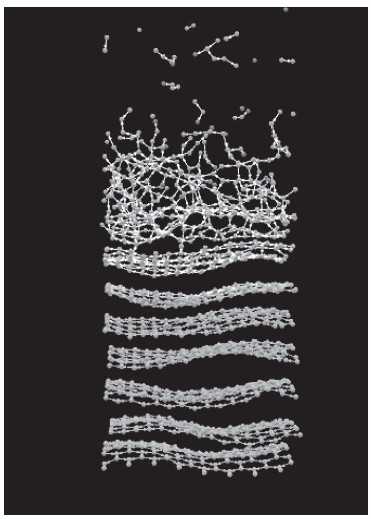

Figure 1: Snapshots of graphene multilayer structure and injected hydrogen atoms in the case that E_{I}=15 eV. The total number of the injected hydrogen atoms n_{H} has increased to 159 and the first graphene sheet contacts with the second one. Thus, the graphene structure is damaged. Fragments of graphene sheets and hydrogen atoms form chain-shaped molecules. The third sheet remains almost unchanged.

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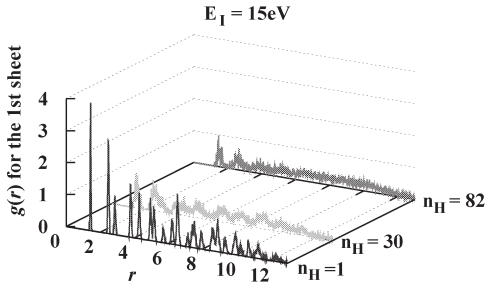
(a)



(b)

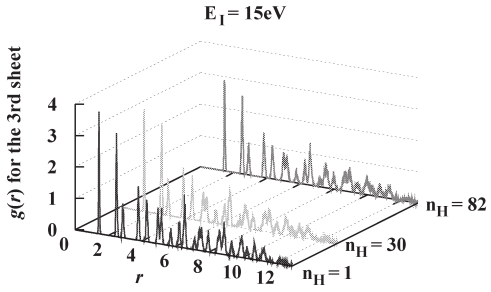


Figure 2: The radial distribution functions $g(r)$ among carbon atoms in the first (a) and the third (b) graphene sheets for the three cases n_{H}=1, n_{H}=30 and n_{H}=82. The incident hydrogen energy is 15 eV.

References

[1] J. Roth, J. Nucl. Mater. **51**, 266–269 (1999).

[2] J. Roth et al. Nucl. Fusion **44**, L21 (2004).

[3] B. V. Mech, et al., J. Nucl. Mater. **1147**, 241–243(1997).

[4] A. Sagara et al. (LHD experimental group), J. Nucl. Mater. **1**, 313–316(2003).

[5] T. Nakano et. al. , Nucl. Fusion **42**, 689 (2002).

[6] D.A. Alman and D.N. Ruzic, J. Nucl. Mater. **313–316**, 182–186 (2002).

[7] A. Ito and H. Nakamura, J. Plasma Phys. **72**, 805–808 (2006).

[8] A. Ito, H. Nakamura and A. Takayama, submitted to J. Nucl. Mater.; e-print cond-mat/0703377.

[9] H. Nakamura and A. Ito, Mol. Sim. **33**, 121–126 (2007).

[10] D. W. Brenner, et al., J. Phys. Condens. Matter **14**, 783 (2002).