§28. The Mechanism of CH_4 Generation in Chemical Sputtering on Graphitic Divertor Plates

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In a nuclear fusion device, divertor plates are bombarded by hydrogen plasma. Then, the divertor plates consist of plasma facing materials (PFM), which are often carbon, tungsten and beryllium. The carbon PFM, which is low-Z material, contributed to achieve high temperature in core plasma. However, since the carbon easily creates chemical bonding with a hydrogen (isotope) atom and ion, the carbon PFM has the problems which are tritium retention, chemical sputtering, chemical erosion, hydrocarbon impurity generation, and its re-deposition. The mechanisms of these chemical processes in the carbon PFM are less well understood. Especially, although a CH_4 molecule is often observed in experiments, its generation process is not clear. In the present work, we clarified the CH_4 generation mechanism by molecular dynamics (MD) simulation.

The MD simulation for chemical sputtering is performed in the following physical system. The graphite composed of 5 layered graphene sheets is put on the center of simulation box, where a graphite (0 0 0 1) surface is facing the positive *z* direction. Each graphene sheet has a size of 20.04 x 21.69 nm^2. The size of simulation box is same to the graphene sheets in the *x* and *y* coordinates where it follows periodic boundary conditions. The graphene sheets are stacked with an ABAB pattern and their interlayer distances are arranged at 3.35 Å. To keep the position of graphite material in the simulation box, six carbon atoms in the deepest graphene sheet are fixed during a simulation. Two kinds of potential models are used. Chemical interaction in short range are represented by modified reactive empirical bond order (REBO) potential.[1,2] To reproduce the layer structure of graphite, the original interlayer intermolecular potential which is created to connect compatibly with REBO type potential by using cone cut-off method.[1] Material temperature is controlled by Langevin thermostat method. Only carbon atoms are following Langevin equation where thermal relaxation time is set to 0.33 ps. Hydrogen atoms with incident energies of 30 eV are injected into the surface normally. Incident flux is 2.5 x 10^{28} -10^{29} atom/m^2s which depends on the transit of the material temperature.

As a result, the CH_4 generation was observed in the present simulation. Note that the MD simulation which did not adopt any thermostat brought about the CH_4 generation hardly. Figure 1 shows CH_x yields after 1500 hydrogen atoms were injected as a function of the material temperature. The CH_4 yield had a peak at 600 K. This peak agrees with experimental results.[3] Especially, the experimental result in the case of low incident energy of less than 100 eV, for example CH_4 yields due to the H^+ injections of 10 and 50 eV[4], is in well agreement. It had been shown by Salonen et al. only that carbon sputtering yield on amorphous carbons indicate a peak at 900 K in MD simulation. Therefore our research could get close to the reality.

To clarify the CH_4 generation mechanism, the reaction path of CH_x was analyzed in the MD simulation. Figure 2 shows the reaction path from detached CH_x to CH_4. From this figure, we can see that dominant process of CH_4 generation is chemical reaction between CH_3 radial and H atom. However, the detachment of CH_3 from surfaces was rare event. In the detachments of CH_x from surfaces, CH is most easily detached. Therefore, we can understand that the dominant path of CH_4 generation as follows: the CH is detached from surfaces and then it grows into CH_4 adsorbing hydrogen atoms via CH_2 and CH_3. From the above result, because CH_4 is always created via CH_3, the CH_3 yield has also a peak at 600 K as well as the CH_4 yield in Fig. 1 can be explained.

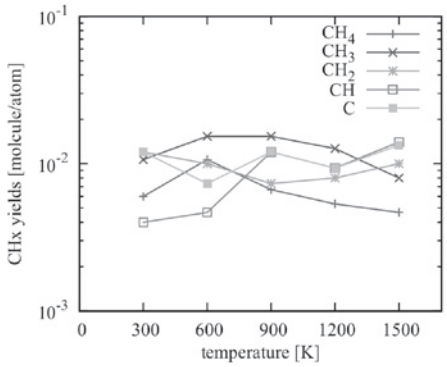

Fig. 1. The CH_4 yields after 1500 hydrogen atoms were injected at 30 eV as a function of material temperature.

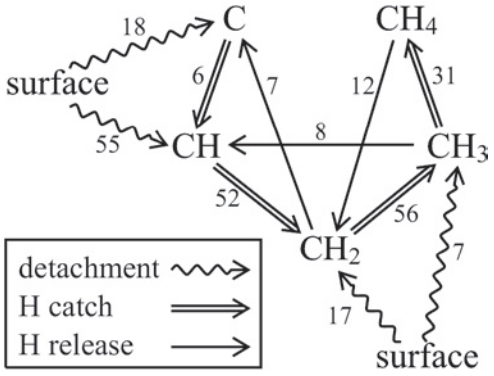

Fig. 2. Reaction path to CH_4 from surfaces. The arrows of wavy line mean the detachment of CH_x from eroded surfaces. The arrows of double and single lines mean the reactions that CH_x catches and releases a hydrogen atom, respectively. The numbers beside the arrows are the numbers of reactions observed in one simulation.

1) Ito, A., et al.: Commun. Comput. Phys. **4** (2008) 592
2) Brenner, D. W., et al.: J. Phys.: Condens. Matter **14** (2002) 783
3) Skinner, C. H., et al.: Fusion Science and Technology **54** (2008) 891
4) Mech B. V., et al.: J. Nucl. Mater. **241-243** (1997) 1147
5) Salonen E., et al.: Phys. Rev. B **63 (**2001) 195415