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Numerical Simulation for Dynamics of Hydrogen Molecules from Inside of Divertor Material to SOL Plasmas

S. Saito[1], H. Nakamura[2,3], K. Sawada[4], G. Kawamura[2,5], M. Kobayashi[2,5], M. Hasuo[6]
[1] Graduate School of Science and Engineering, Yamagata University,
[2] Department of Helical Plasma Research, National Institute for Fusion Science,
[3] Graduate School of Engineering, Nagoya University,
[4] Interdisciplinary Graduate School of Science and Technology, Shinshu University,
[5] Department of Fusion Science, The Graduate University for Advanced Studies, SOKENDAI,
[6] Graduate School of Engineering, Kyoto University
e-mail (speaker): saitos@yz.yamagata-u.ac.jp

When the divertor plates are irradiated by hydrogen plasma, some hydrogen atoms and molecules reflect and back to the plasma while the other hydrogen retain in the divertor. In addition to the investigation of this recycled hydrogen atoms, that of hydrogen molecules at the divertor is an important issue because this recycled hydrogen molecules affect the plasma parameter by molecular assisted recombination (MAR). The rate coefficients of the MAR processes strongly depend on both vibrational and rotational states of hydrogen molecules.

The transport of the neutral particles can be numerically simulated by Neutral-Transport code with the rovibrationally resolved Collisional-Radiative model (NT-CR) code. Although both vibrational and rotational states strongly affect the rate coefficients of MAR, most of conventional code only distinguish the vibrational state. To solve this situation, Shinshu University group is developing a new NT-CR code which distinguish their rotational states in addition to the vibrational states. In this study, therefore, in order to provide information of recycled hydrogen atoms and molecules on the divertor to NT-CR code, molecular dynamics (MD) simulation of a hydrogen atom injection into carbon and tungsten material is performed to investigate the distribution of the rovibrational states, translational energy and emission angle of emitted hydrogen molecules in addition to atoms.

Figure 1(a) shows our MD simulation model [1, 2] for carbon divertor. Blue and black balls denote the carbon and hydrogen atoms, respectively. One hydrogen atom is injected into a hydrogen contained amorphous carbon material from the height of 10 Å from the surface of amorphous carbon. Incident energy is set to 100 eV. The initial material temperature is set to 300 K. The motion of atoms is calculated for 50 ps after injection of a hydrogen atom. Then the information of hydrogen atoms and molecules released are observed during the simulation is running. Figure 1(b) shows one of the examples of the emission process. A hydrogen molecule and a hydrocarbon are emitted as a result of breaking the chemical bonds by incident hydrogen atom. By repeating the same simulation with randomly selected incident positions, the distributions of emission angle, the translational energy, and the rotational and vibrational states are obtained.

Figure 2 shows the obtained distribution of rotational state of emitted hydrogen molecules from the material. It is found that molecules with relatively high rotational state are generated. The simulation result shows that some hydrogen molecules are also in high vibrational state. And it is revealed that such molecules which have high rotational and vibrational states emit within 1 ps after the injection.

The all distributions obtained by developed MD model is successfully provided to a NT-CR simulation discussed in Ref. 3. In our presentation, we would like to explain the results of the NT-CR calculation with developed MD model. Also, we would like to discuss the hydrogen recycling process in the case of tungsten material.

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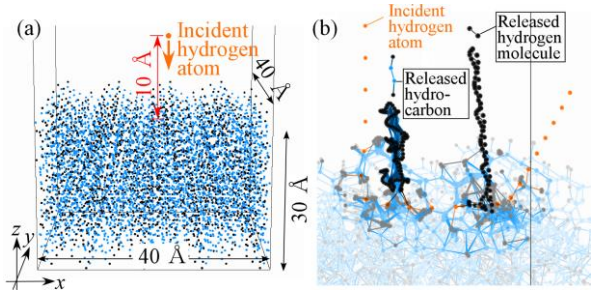

Fig. 1 (a) MD simulation model for carbon divertor. (b) One of the examples of the emission process of a hydrogen molecule.

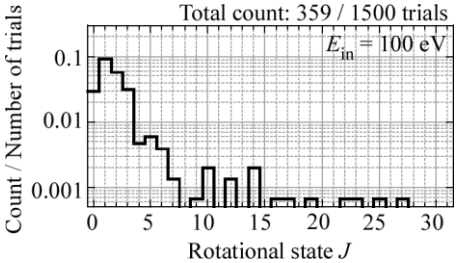

Fig. 2 Distribution of rotational state of emitted hydrogen molecules from carbon divertor.

References

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