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# Emission of high rovibrational molecules from tungsten divertor

S. Saito[1], H. Nakamura[2], S. Sawada[2], K. Hoshino[2],
M. Kobayashi[2], M. Hasuo[2], Y. Homma[2], and S. Yamoto[2]
[1] Yamagata University, Yonezawa, Japan
[2] National Institute for Fusion Science, Toki, Japan
[3] Nagoya University, Nagoya, Japan
[4] Shinshu University, Nagano, Japan
[5] Keio University, Yokohama, Japan
[6] Kyoto University, Kyoto, Japan
[7] National Institutes for Quantum and Radiological Science and Technology, Rokkasho, Japan
[8] National Institutes for Quantum and Radiological Science and Technology, Naka, Japan
e-mail (speaker): saitos@yz.yamagata-u.ac.jp

## 1. Introduction

In the case of detached plasma, Molecular Assisted Recombination (MAR), such as charge exchange and dissociative recombination (DAR), plays a significant role in the particle transport within the edge plasma. It is widely recognized that the rate coefficient of MAR can vary by several orders of magnitude depending on the rovibrational states of hydrogen molecules.

Hydrogen molecules are produced on the wall through the hydrogen recycling process. While there is a possibility that the hydrogen molecules generated on the wall could impact MAR in the edge plasma, this process has not been thoroughly investigated yet due to the difficulties in experimentally determining the rovibrational states of these hydrogen molecules. In this paper, therefore, we employ a molecular dynamics simulation [1-4] to estimate the rovibrational states of recycled hydrogen molecules on the tungsten divertor in the DEMO reactor under detached plasma conditions. Subsequently, we utilize a neutral transport code [5], developed by Prof. Sawada's group, incorporating the information regarding the generated molecules on the wall obtained from the MD simulation.

## 2. Simulation Results

The simulation results [6] reveal that molecules in high rovibrational states are emitted even in cases of low incident energy, which are expected to be the dominant conditions during detached plasma. Figure 1 illustrates the distributions of rotational states for emitted hydrogen molecules under various incident energy conditions. It is evident that certain molecules exhibit high rotational states, even in scenarios involving low incident energy injection.

The trajectory analysis of the simulation reveals the emission mechanism as follows: 1. In cases of low incident energy, the incident hydrogen atom is unable to penetrate the target material. 2. The incident atom becomes trapped at the surface due to the influence of surface binding energy. 3. The incident atom traverses the surface until it comes into contact with other hydrogen atoms situated on the surface. 4. Upon contact with these other hydrogen atoms, a hydrogen molecule is formed, subsequently detaching from the surface.

To clarify the effects of such emitted hydrogen molecules from divertor of DEMO reactor, we also develop a neutral transport simulation in edge plasma with the emission distributions by MD simulation for the divertor. As shown in Figure 2, the distribution of rotational states for hydrogen molecules in the edge plasma, situated 2 cm from the divertor, demonstrates the presence of molecules exhibiting high rotational states.

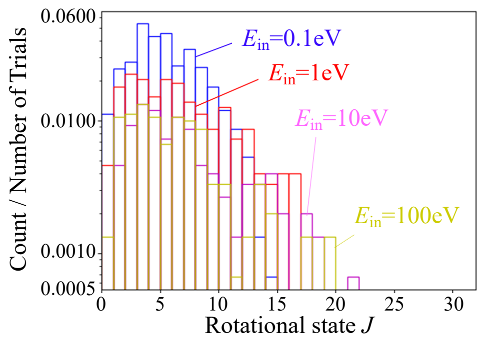


Figure 1 Distributions of rotational states of emitted hydrogen molecules from tungsten divertor.

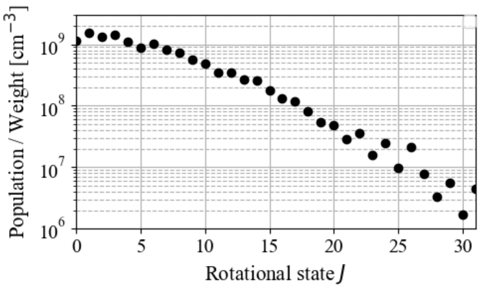


Figure 2 Distribution of rotational states of edge plasma near the divertor obtained by neutral transport simulation.

## References

[1] S. Saito, et. al., Contrib. Plasma Phys. e201900152 (2020).
[2] S. Saito, et. al., Plasma Fusion Res. 15, 2403073 (2020).
[3] S. Saito, et. al., Jpn. J. Appl. Phys. 60, SAAB08 (2021).
[4] H. Nakamura, S. Saito, et. al., Jpn. J. Appl. Phys. 61, SA1005 (2022).
[5] K. Sawada, S. Saito, et. al., Contrib. Plasma Phys. e201900153 (2020).
[6] S. S. Saito, et. al., Synopsis of IAEA-FEC 2023, Contribution ID: 1733, https://conferences.iaea.org/event/316/contributions/28538/