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MD simulation with deep learning on ro-vibrational population of hydrogen isotopologues for neutral transport analysis

Hiroaki Nakamura[1,2], Seiki Saito[3], Keiji Sawada[4], Masahiro Hasuo[5], Masahiro Kobayashi[1]
[1] National Institute for Fusion Science, [2] Graduate School of Engineering, Nagoya University, [3] Graduate School of Science and Engineering, Yamagata University, [4] Faculty of Engineering, Shinshu University, [5] Graduate School of Engineering, Kyoto University
e-mail (speaker): hnakamura@nifs.ac.jp

The detached plasma is one of the expected phenomena to decrease the heat flux to the divertor plate. It is pointed out that the molecular assisted recombination (MAR) may play a significant role in the detached plasmas. To analyze the MAR, Sawada, et al. developed the Neutral-Transport code including the rovibrationally resolved Collisional-Radiative model, (NT-CR code)[1].

In the NT-CR model, the reaction rate coefficients of H_2 in the divertor plasmas strongly depend on the initial rovibrational state of H_2. We calculated the rovibrational state distribution of the released H_2 or its isotopologues from carbon by MD simulation[2,3]. Using these data, we evaluated the rovibrational population produced in the LHD plasma as Fig.1 and 2[4].

Moreover, we also calculated the distribution of the hydrogen isotoplogues from graphite as shown in Fig. 3 [3,5]. From these simulations, we learned the hard way that a lot of statistics need to be taken, which requires an enormous amount of computation time. To overcome this problem, we attempted to use deep learning method to obtain the distributions of the hydrogen isotopologues.

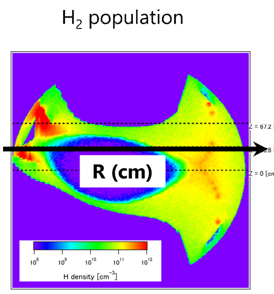

Figure 1 Hydrogen molecules distribution of LHD.

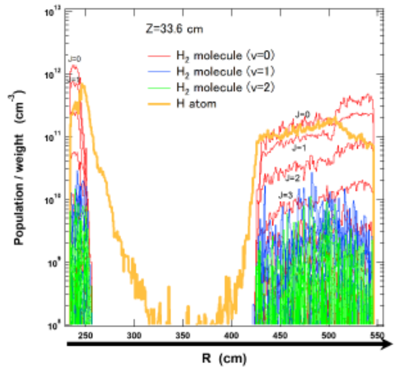

Figure 2. R-dependence of hydrogen molecule population for vibrational levels v = 0, 1, 2.

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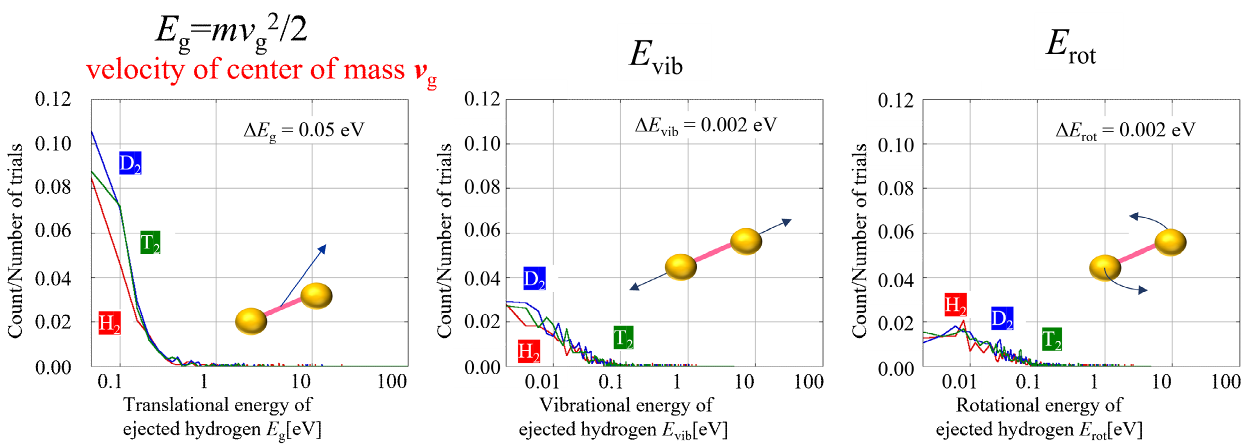

Figure 2 Population of hydrogen isotopologues (H_2, D_2, and T_2) for three energies, i.e., Translational energy (E_g), vibrational energy (E_{vib}), and rotational energy (E_{rot}).