Molecular dynamics simulation on energy distribution of hydrogen isotopes generated from carbon and tungsten

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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 plasma[1]. To analyse the MAR, we developed the neutral-transport code including a rovibrationally resolved collisional-radiative (CR) model of molecular hydrogen[2]. In the CR model, the reaction rate coefficients of molecular hydrogen in the divertor plasmas strongly depend on the initial rovibrational state of the molecules[2]. We calculated the rovibrational state distribution of the released molecules from carbon by molecular dynamics (MD) simulation[3,4]. Using these data, we evaluated the rovibrational population produced in the LHD plasma. In the divertor plasma region, it was found that the initial higher rotational state molecules were lost by the dissociative attachment of the electron[3]. Thus, we succeeded in calculating the spacial distribution of hydrogen molecules and atoms combining the neutral-transport code including CR model with the MD simulation for carbon material[3,4]

Based on the previous MD simulation of carbon material, we try the MD simulation of the hydrogen isotope effect as in Fig. 1. We also calculate the hydrogen isotope effects of tungsten as well as carbon as in Fig.2.

[3] K. Sawada et al., 17th PET, 19-21 August, 2019, USA. ; submitted to CtPP.