Calculation of D/XB values of hydrocarbon molecules in tokamak edge plasmas

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In a next-step magnetically confined fusion devices, such as ITER, it is very important to estimate lifetime of plasma-facing components in which are made with carbon-based materials. And to reveal a process of chemical erosion of the facing components via formation of hydrocarbon molecules is a crucial issue. In many recent tokamaks, chemical sputtering yields are experimentally measured by spectroscopic method using inverse photon-efficiency D/XB. Photon fluxes are converted into particle fluxes with aid of effective D/XB values, and effective D/XB values are critical factors in the study of chemical erosion by spectroscopic measurements.

In this study, effective D/XB values of hydrocarbon molecules (CD_4, $C_2D_x(x = 2,4,6)$, $C_3D_y(y = 4,6,8)$) for CD and C_2 emissions have been calculated by a Monte Carlo simulation. In a simple modeled divertor plasma region with the constant temperature and density, hydrocarbon transport are simulated [1]. The CD Gerö band and C_2 Swan band emission intensities are calculated in a condition of corona equilibrium. The complex dissociation and ionization reactions of hydrocarbon molecules and the surface reflection process are taken into account. The simulation volume is $10 \times 10 \times 10$ cm^{-3}. The angle of the magnetic field lines with the toroidal direction is 5° and the lines are inclined by 30° against the poloidal direction. The magnetic filed strength is 5 T. The hydrocarbon molecules are released at the center of the divertor plate with a Maxwellian velocity distribution corresponding to a temperature of 0.1 eV (1160 K). The released particle number is 10^5.

In the condition of the multiple reflection at the divertor surface and the plasma density of 1.0×10^{19} m^{-3}, the calculation of the temperature dependence of effective D/XB values, for CD and C_2 from methane (CD_4), ethane family (C_2D_2,C_2D_4,C_2D_6) and propane family (C_3D_4, C_3D_6, C_3D_8), has been performed. The D/XB values decrease with increasing the temperature up to 5 eV and then these increase with the temperature caused by decrease of number of hydrocarbon fragments, which are produced by dissociation processes, of type CD and C_2. In the comparison with experimentally determined values [2], a good agreement is obtained for CD emission in the region in which the plasma temperature is higher than 25 eV. On the other hand, for C_2 emission, there are qualitative agreements. But experimental values are several times larger than those of the calculated.

[1] K. Ohya, et. al., J. Plasma. Fusion Research Series, in press.
[2] A. Pospieszczyk, et. al., Report UCLA-PPG-1251 (December 1989).