Molecular Enhanced Recombination in the Divertor of ASDEX Upgrade

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Abstract. The contribution of hydrogen molecules to plasma recombination in the ASDEX Upgrade Lyra divertor was investigated by combining optical emission spectroscopy and B2-EIRENE calculations. Measured and predicted Fulcher band photon fluxes are in good agreement, provided that the vibrational levels in the ground state are included as distinct particles and a collisional radiative (CR) model is applied for the density dependence of the emission rate coefficient. The vibrational population in the ground state was gained from measurements and the CR-model. In space resolved calculations of the molecular enhanced recombination (MAR) and competing processes, the populations have to be considered. The integrated results give a minor effect of MAR in the divertor. MAR is decreased by the molecular assisted dissociation, being the dominant reaction channel for the hydrogen molecules. However, near the surfaces the contribution of MAR is comparable with the three-body and radiative recombination.

1. Introduction

Vibrationally excited hydrogen molecules are responsible for the MAR process. Two reaction channels can contribute to this kind of plasma recombination: The ion conversion channel ($H_2(v)$ + $H^+ \rightarrow H_2^+$ + H followed by H_2^+ + e $\rightarrow$ H* + H) is dominant in comparison with the negative ion channel ($H_2(v)$ + e $\rightarrow H^-$ + H followed by H^- + $H^+ \rightarrow$ H* + H) [1, 2]. Considering the effect of ionization of the excited hydrogen atoms produced by the ion conversion channel, the enhanced recombination factor was found to be three [1], based on calculations with plasma parameters supposed to be typical for detached divertor plasmas. Previous spectroscopic investigations have shown remarkable population of the vibrational levels and molecular hydrogen fluxes, which were in the range of the atomic hydrogen fluxes [3], especially in the detached divertor plasma.

In this paper, the contribution of the molecular enhanced recombination in the divertor of ASDEX Upgrade to the plasma recombination (three-body and radiative recombination R^{3+r}) was determined combining measurements of the Fulcher photon flux and the vibrational population in the ground state with results of the B2-EIRENE code. For a detailed evaluation, the collisional radiative model of Sawada and Fujimoto [4] was used, extended by some selected reactions. This CR-model was also applied for rate coefficients, necessary for calculations of the three competing processes which can occur after the ion conversion reaction: H_2^+ + e $\rightarrow$ H + H (molecular enhanced recombination MAR), H_2^+ + e $\rightarrow H^+$ + H + e (molecular assisted dissociation MAD) and H_2^+ + e $\rightarrow H^+ + H^+$ + 2e (molecular assisted ionization MAI).

2. Method

From measurements of the diagonal Fulcher band emission ($d\ ^3\Pi_u \rightarrow a\ ^3\Sigma_g^+$, v'=v''=0,1, around 600 nm) the hydrogen flux and the vibrational population in the ground state were obtained in the

divertor of ASDEX Upgrade [3]. Both show a weak dependence on the lines-of-sight, which is not further interpreted here, but a strong time dependence, which is due to the transition from the attached to the detached plasma. In the detached case the measured molecular fluxes ($\Gamma_{H2} = 10^{22}$ $m^{-2}s^{-1}$) are in the same order of magnitude as the ion fluxes, which were obtained from probe measurements and the atomic hydrogen fluxes ($\Gamma_H = 4\text{-}8 \times 10^{22}$ $m^{-2}s^{-1}$) derived from the H_β-line. The diagnostic method for the determination of vibrational population in the ground state [5] was improved by using predicted vibrational population in the ground state of the hydrogen molecule from the extended CR-model. The original version of the CR-model has been extended by vibrationally resolved electronic excitation in the first excited electronic states (B $^1\Sigma_u^+$, C $^1\Pi_u$ - states of H_2) [6] followed by radiative decay leading to a stronger population of higher vibrational levels (v>4). The rate coefficient for dissociation of the molecule via the repulsive b $^3\Sigma_g^+$ state was

exchanged for new vibrationally resolved rate coefficients for dissociation [7], leading to a decrease in the vibrational population. The non-thermal populations were transferred in the upper Fulcher state d $^3\Pi_u$, assuming Franck-Condon excitation, showing a steep dependence on electron temperature in the range of 2 - 10 eV. The comparison of the predicted upper state populations with the measured ones agree very well.

Fig. 1: Geometry of the ASDEX Upgrade divertor with the grid of B2-EIRENE code. Zoomed is the region of the lines-of-sight.

Calculations with the B2-EIRENE code were carried out considering in EIRENE the vibrational states of the molecule (v=0-7) as distinct species leading to a smaller molecular hydrogen density (factor three). In addition, the influence of various wall effects has been tested: case a) the molecules start with v=0 at the wall, case b) recombined ions result in v=0 and recombined atoms and molecules in v=2, case c) recombined ions and atoms contribute to molecules in v=3 and molecules come back with v=0. For comparison with measurements, these cases have been calculated for the parameters of a detached and an attached divertor plasma. Figure 1 illustrates the geometry of the Lyra divertor and the grid of the B2-EIRENE code. Zoomed are the lines-of-sight which were used for measurements. The application of the collisional radiative model allows predictions of the Fulcher radiation. The

molecular density, n_e and T_e were taken from the code integrated over a line-of-sight. Using the extended CR-model, the emission rate coefficient for these plasma parameters was calculated. A strong decrease of the rate coefficient with increasing electron density was observed, which is more than one order of magnitude from $n_e = 10^{18}$ m^{-3} to $n_e = 10^{20}$ m^{-3}, typical for divertor plasmas. Figure 2 shows the good agreement between the measured and calculated Fulcher photon fluxes, which can only be obtained by using the electron density dependence of the Fulcher rate. A comparison of B2-EIRENE results with
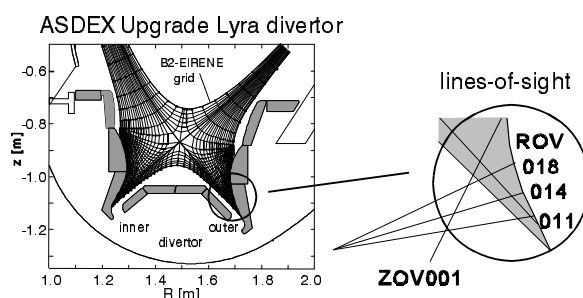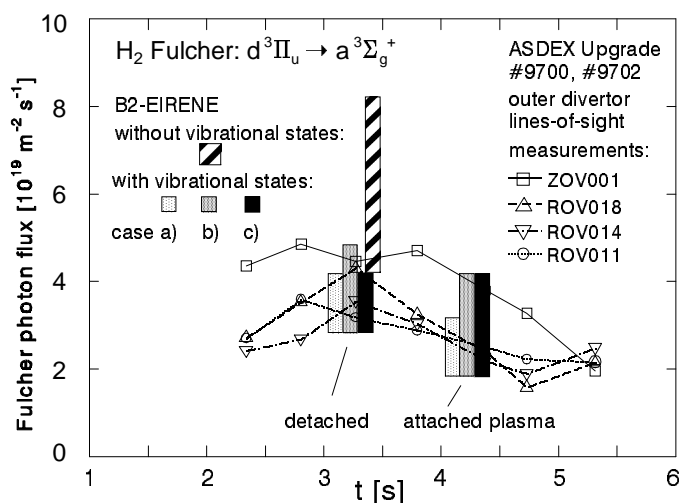

Fig. 2: Measured Fulcher photon flux depending on time for various lines-of-sight in comparison with B2-EIRENE results.

and without treating the vibrational levels as separate particles, reproduces the influence of the decreased molecular density. However, the photon flux is not a criterion to distinguish the various cases assumed for the wall effect on the $H_2(v)$ population.

3. Results

The vibrational population predicted from the CR-model and confirmed by the measurements was compared with the populations calculated with the B2-EIRENE code for one line-of-sight (Fig. 3). Both methods give a significant vibrational population in the ground state in the detached and in the attached divertor plasma. Case a) from the B2-EIRENE calculation leads to the best agreement with measurement e.g. molecules start without vi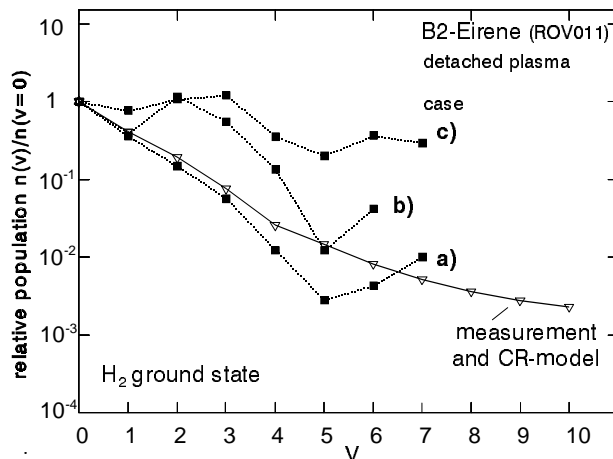brational population from the wall. Case c) shows a strong increase of the population and a peak at v=3 caused by the high ion flux to

Fig. 3: Vibrational population in the ground state of hydrogen. Measurements and calculations assuming various wall effects.

the wall. Case b) shows the peak at v=2 with a decrease to higher levels. On the basis of our measurements case b) can be excluded, because the vibrational population in the upper state transfered from this ground state population achieves values which were not obtained. In spite of the different population in the ground state, case a) and c) result in a very similar relative population for the measured v'=1/v'=0 ratio in the upper Fulcher state.

The contribution of the hydrogen molecules to the plasma recombination was calculated using the densities from the B2-EIRENE code, especially the molecular density including vibrational population. Rate coefficients for the predicted plasma parameters (n_e, T_e) were taken from the CR-model. The ion conversion channel dominates the negative ion channel because the reaction rate of the ion conversion reaction is high at low T_e and shows a strong increase with vibrational population. As mentioned before, there is a distinction between the possibilities after the ion conversion reaction. The rates for these processes (MAR, MAD, MAI) are given by the rate coefficients multiplied with the corresponding densities. Figure 4 shows these three rates resolved

along a line-of-sight in comparison with the rate for the three-body and radiative recombination R^{3+r} of the hydrogen ions H^+ in the detached plasma. Choosen was ROV011 with a length of 2 cm the lowest part of the outer Lyra divertor and case a) of the wall influences. The dominant process is the molecular assisted dissociation, which reduces dramatically the reaction channel for the molecular enhanced recombination. MAR is of the order of the three-body and radiative recombination near the walls decreasing nearly two orders of magnitude below R^{3+r}. The molecular assisted ionization is
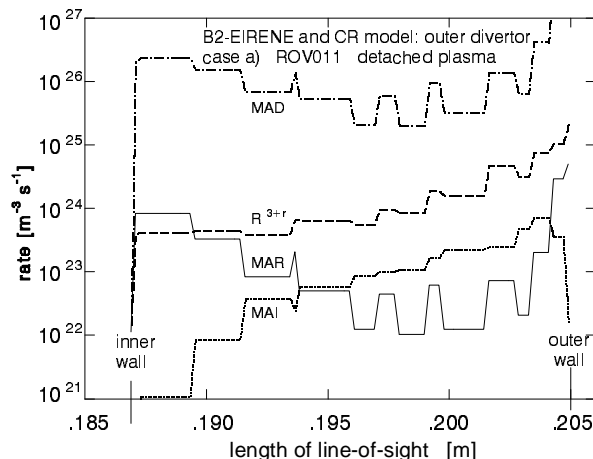

Fig. 4: Line-of-sight resolved rates calculated with B2-EIRENE including the CR- model for hydrogen.

getting important at the outer region. The atomic hydrogen density is in the range of 10^{21}-10^{22} m^{-3}, the electron temperature between 2 and 5 eV, both increasing from the inner to the outer zone. Near the walls, the molecular density is higher than the atomic density, decreasing between the walls to 10^{20} m^{-3}. These plasma parameters, together with a high rate coeffcient for the molecular assisted dissociation 10^{-14}-10^{-13} m^3 s^1, lead to the strong contribution of MAD. The various cases calculated for the effect of the walls on the vibrational population give no remarkable difference in the results shown in Fig.4.

4. Conclusions

The vibrational population of the hydrogen molecules has to be considered in the calculations of B2-EIRENE leading to a good agreement with the measured photon flux together with the usage of the electron density dependence of the Fulcher rate coefficient taken from the CR-model for hydrogen. This model was extended, the vibrationally resolved rate coefficients have a clear influence on the vibrational population in the ground state, being in good agreement with measurements gained from the emission spectroscopy of the Fulcher transition. The diagnostic method for the vibrational population was improved, giving information about more vibrational levels. For the different wall effects on the vibrational population of the molecules assumed in the B2-EIRENE code case a) and c) fit to measurements, whereas case b) can by excluded. More likely than a distinct population of one level at the wall, would be the assumption of a vibrational temperature around 3000 K (caused be recombined atoms), given in literature for some metals [8]. Results of hydrogen discharges and modeling lead to wall-relaxation processes of the vibrationally excited molecules, decreasing in prinicple the population of the H$_2$(v) particles by one quantum number after each contact with the wall [9]. For a better statement about the wall effect on the vibrational population more vibrational levels of the Fulcher transition have to be measured and compared with results from B2-EIRENE.

The results from measurements and calculations confirm the minor effect of molecular enhanced recombination in the divertor plasma integrated over a line-of-sight. The integrated molecular density is smaller than the atomic density and even decreased by the ionization of excited hydrogen atoms in the ion conversion channel. This molecular assisted dissociation is the most important reaction occuring in these processes. Space resolved calculations along a line-of-sight give a contribution of MAR comparable with the plasma recombination in the regions near the wall.

Concerning deuterium plasmas the methods introduced have to be tested. Rate coefficients for reactions may differ for hydrogen and deuterium, due to the lower lying vibrational levels. Therefore, the CR-model has to be changed to deuterium, but there is a lack of data, especially concerning vibrationally resolved rate coefficients. The B2-EIRENE code uses a hydrogen model, which is valid for both atoms.

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