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Optical emission measurements of H_2 and D_2 molecules in the divertor region of ASDEX Upgrade

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Abstract

A spectroscopic method has been developed for measuring molecular influxes and particle densities in fusion edge plasmas, which is based on the H_2 and D_2 Fulcher emission bands around 600 nm wavelength. A first application to the ASDEX Upgrade divertor plasma is described. The influx of hydrogen molecules was determined from the population of the upper Fulcher state using the theoretical number of ionization and dissociation events per Fulcher photon $(S_{\mathrm{eff}} + D_{\mathrm{eff}})/XB_{\mathrm{Ful}}$, as calculated by a collisional-radiative model. These results were compared with expectations on the basis of the atomic hydrogen fluxes and a typical molecule/atom ratio. Measurements and calculations agree in their time dependence, but the experimental values are somewhat lower, which may be within the error margin or of more significance. The Fulcher radiation was also compared directly to B2-EIRENE predictions, resulting in a higher discrepancy. In addition, the vibrational population of the ground state molecules was determined from that of the excited state using a method based on Franck–Condon factors. It can be characterized by a T_{vib} between 3000 and 9000 K, inversely correlated with electron temperature. This variation is predicted by the collisional-radiative code and even allows an estimate of T_e. Vibrational excitation increases ionization and dissociation rate coefficients, as clearly demonstrated by the code calculations. It is therefore very likely that the observed discrepancy in molecular intensity is mainly caused by the omission of vibrational excitation in the present version of B2-EIRENE. The described flux measurements are expected to be accurate above $T_e = 5$ eV, but are more difficult at lower temperatures due to the strong T_e dependence of $(S_{\mathrm{eff}} + D_{\mathrm{eff}})/XB_{\mathrm{Ful}}$ in that region. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Knowledge of hydrogen and deuterium molecular densities, fluxes and ground state vibrational excitation is required for a better understanding of the role of these molecules in the recombination of divertor plasmas [1,2]. The molecular enhanced recombination is predicted to occur in detached divertor regimes, which are characterized by low electron temperatures near the divertor plates together with a decrease in plasma particle flow velocity. The vibrationally excited molecules [$H_2(v)$, $D_2(v)$] increase plasma recombination due to dissociative attachment $H_2(v) + e \rightarrow H^- + H$ followed by mutual neutralization $H^- + H^+ \rightarrow H + H^*$ and ion conversion $H_2(v) + H^+ \rightarrow H_2^+ + H$ followed by dissociative recombination $H_2^+ + e \rightarrow H + H^*$, where the latter channel is found to be dominant [1,2]. Considering re-ionization of the resulting electronically excited state (H^*) and the decay into the ground state the enhanced recombination factor was found to be 3 [1].

A spectroscopic method is presented here for measuring hydrogen molecular influxes and particle densities from the intensities of the H_2 and D_2 diagonal Fulcher bands. For this purpose, the number of ionization and dissociation events per Fulcher photon has been calculated by a collisional-radiative model [3,4]. The relative strengths of the Fulcher vibrational branches represent an additional diagnostic tool for measuring

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the vibrational population of the ground state, i.e. in v'', projected up into the electronically excited state according to the Franck–Condon principle. This method gives reliable results up to $v'' \approx 4$, for higher v'' it becomes insensitive due to the low population of those highly excited states. The vibrational distribution can also be predicted by the collisional-radiative model as a function of T_e, which can thus be derived from the measured spectra.

2. Method

The emission of the Fulcher band ($d^3\Pi_u \rightarrow a^3\Sigma_g^+$) in the divertor plasma of ASDEX Upgrade was measured by means of a 1 m spectrometer and a CCD camera providing a spectral resolution of 0.05 nm. Spatial resolution was achieved by a fibre-optical system described by Gafert et al. [5], using only the poloidal lines-of-sight (LOS). Since the mass of the molecules is rather small, the spectrum appears as a multi-line spectrum. In the wavelength range of the Fulcher transition (between 590 and 640 nm), the individual vibrational transitions ($v' = v'' = 0$–4) partly overlap and are disturbed by lines from plasma impurities. Nevertheless, this transition is the only candidate with sufficient intensity in divertor plasmas. The spectroscopic system allows the measurement of a wavelength range of 7.7 nm per plasma pulse. For analysis of the rotational and vibrational population of the upper Fulcher state ($d^3\Pi_u$), the rotational lines of various vibrational transitions were recorded during identical shots with shifted wavelength windows.

The rotational temperature was determined from the Q branch (Q1–Q5) using a Boltzmann plot resulting in lower rotational temperatures for higher vibrational transitions (e.g. 0-0 transition: 3000–8000 K, 1-1 transition 1500–2000 K for H_2 and D_2). Using T_{rot}, the relevant statistical weigths and the Hönl–London factors (theoretical line strengths), the intensity of the Q branch was derived from the measured lines and subsequently, the R- and P-branches were added to get the total emission in the vibrational transition. These integrals allow analysis of the relative vibrational population of the upper state on the basis of their branching ratios. Assuming the validity of the Franck–Condon principle for electron impact excitation, the upper vibrational levels are populated from the ground state ($X^1\Sigma_g^+$) according to the corresponding Franck–Condon factors. For the present analysis, the relative population of the lower vibrational ground state levels was characterized by a temperature T_{vib}, used as a parameter in the comparison between a calculated and measured upper Fulcher state vibrational population. A detailed description of this diagnostic method is given in Ref. [6], together with experimental results in low pressure H_2 and D_2 plasmas verifying the underlying assumptions. The relative distribution of the ground state vibrational levels can be determined up to $v'' = 4$ with acceptable error bars. Analysis of the upper Fulcher state is limited to $v' = 3$ in H_2 and $v' = 4$ in D_2 due to pre-dissociation.

The vibrational population of the ground state was also calculated using the collisional-radiative model of H_2 and H from Sawada and Fujimoto [3], extended by Reiter and Greenland [4]. In the original version only electron collisions were taken into account for the population and de-population of the vibrational states, the dominating processes in divertor plasmas. The model was extended by electronic excitation into the B and C states in the singlet system followed by radiative decay, which leads to a pronounced non-thermal distribution for vibrational levels $v'' > 4$. The model calculations predict a correlation between the vibrational population, still characterized by T_{vib} for lower v'', and the electron temperature, as shown in Fig. 1. In the range of 3–10 eV, T_{vib} decreases, whereas it is nearly constant between 1–3 eV.

For molecular influx measurements, the total population of the upper Fulcher state is required, i.e. the sum over rotational and vibrational levels, as well as the theoretical number of ionization and dissociation (via the repulsive triplet state) events per Fulcher photon. The total Fulcher emission cross section is given in Ref. [7]. Since only part of the vibrational transitions was measured, the appropriate theoretical ratio must be applied (e.g. 1.09/4.2 for 0-0 and 1-1 transitions only [7]). The effective ionization rate coefficient S_{eff} and the dissociation rate coefficients D_{eff} were calculated again by the collisional-radiative model for H_2 [3] with and without taking into account vibrational excitation, as shown in Fig. 2. The ion conversion ($H_2(v) + H^+ \rightarrow H_2^+ + H$) is the main reaction which leads to an increase in the ionization rate coefficient at low T_e, when including vibrational excitation. The increase in the dis-

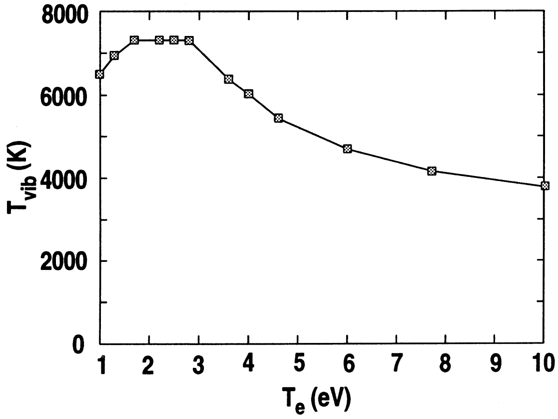

Fig. 1. Calculated vibrational population of the ground state of H_2 characterized by T_{vib} up to $v'' = 4$.

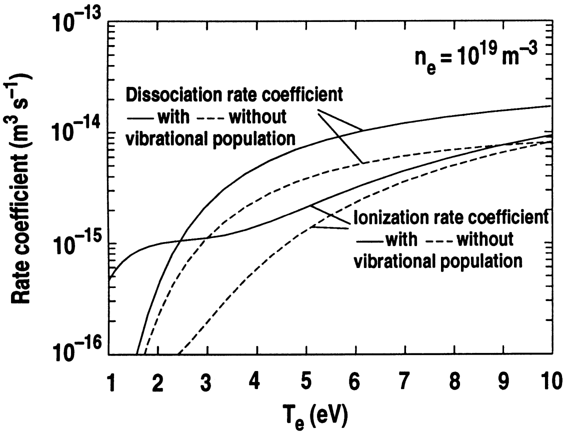

Fig. 2. Rate coefficients with and without vibrational population calculated using the collisional-radiative model [3].

sociation rate is due to the threshold energy (8.3 eV) and the reduction of approximately 0.5 eV per vibrational level for H_2. In Fig. 3, the theoretical number of ionization and dissociation events per emitted Fulcher photon (S_{eff} + D_{eff})/XB_{Ful} is presented. Again, coefficients with and without vibrational excitation in the ground state are shown, as well as the ones with ionization alone. For measurements of the molecular flux, (S_{eff} + D_{eff})/XB_{Ful} must be applied with all effects included. As can be seen in Fig. 3, this method for determining the hydrogen molecular influxes is very suitable for the temperature range above 5 eV, because (S_{eff} + D_{eff})/XB_{Ful} is nearly constant ($\approx$100). For temperatures lower than 5 eV the ratio rises due to the fact that the dissociation threshold of 8.3 eV is lower than the excitation threshold of the upper Fulcher state (13.97 eV). This becomes even more important for $T_e < 3$ eV together with the increase of ionization by ion conversion at low energies. For the diagnostics of cold divertor plasmas, the temperature of the plasma region, where the Fulcher emission originates, must be accurately known.

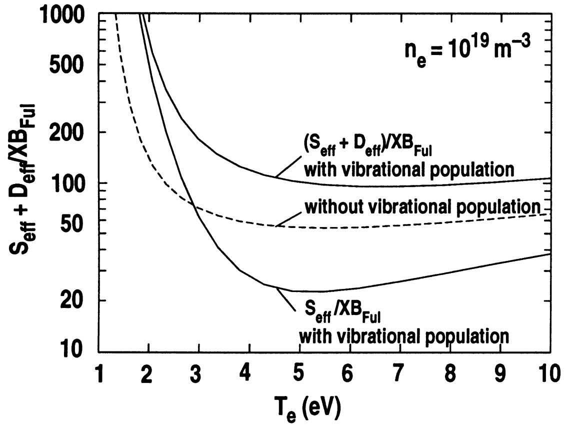

Fig. 3. Theoretical number of ionization and dissociation events per emitted Fulcher photon.

The influx of H_2 molecules was also determined from the R-branch of the 0-0 singlet transition G $^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ around 463 nm (slightly disturbed by the CIII line at 465 nm). However, the intensity of this band is very low. The cross section is given in Ref. [8]. For D_2 this band is close to the very strong CIII line and is therefore not suitable for measurements.

3. Results and discussion

ASDEX Upgrade plasma pulses were investigated, which are characterized by relatively high densities and a detached inner divertor (LYRA divertor). The plasma in the outer divertor was still attached, except for the time interval between 3.2 and 3.8 s. The poloidal LOS were above the strike point in the inner and outer divertor region (geometry and description is shown in Ref. [5]). Molecular intensities are spread out over many individual lines and were generally found to be low. This is due to the relatively high dissociation rate coefficients even at low T, leading to small molecular densities in the region of electronic excitation. Thus, the inner divertor signals were too small to be analyzed. The plasma parameters in the outer divertor region, as measured by probes, were $T_e = 5$–15 eV, $n_e \approx 4 \times 10^{19}$ m^{-3}. For the completely detached case, analysis of the Paschen and Balmer continuum radiation [9] resulted in T_e between 1 and 10 eV and in n_e about 2–5 × 10^{20} m^{-3}.

In the measured spectra, the rotational temperatures in the excited state ($d^3\Pi_u$) varied strongly with vibrational level, and were $T_{rot} \approx$ 2000–8000 K ± 50 K (0-0 band), 1500–2000 K (1-1 band) for H_2 depending on time, but little on LOS. This confirms the necessity for measuring many individual lines with high enough spectral resolution. The vibrational temperatures in the H_2 ground state were found to be $T_{vib} = 3000$–9000 K ± 500 K depending on LOS and time, as shown in Fig. 4. Because of the wide spectral range of the emission bands only two vibrational transitions could be analyzed in two shots, resulting in relatively high error bars for T_{vib}. For $T_{vib} > 9000$ K the sensitivity of the method is very low and, considering the limited accuracy, an assignment of T_{vib} becomes difficult. It was therefore set to 9000 K in Fig. 4. As an example, a T_{vib} of 5000 K in the ground state of H_2 means a population of 71%, 20%, 6%, 2% for the levels $v'' = 0$, 1, 2, 3, respectively. Nearly the same population results for $T_{vib} = 3000$ K in D_2, due to the lower energy separation of the vibrational levels. According to the model calculations, T_{vib} is expected to be >7500 K at $T_e = 2$–3 eV, and to decrease to 4000 K at 10 eV for H_2 (Fig. 1). It is

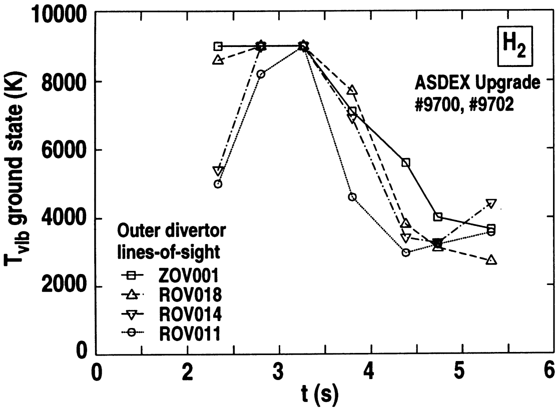

Fig. 4. Measured vibrational temperature in the ground state depending on time and LOS.

therefore concluded that the measured range of vibrational temperatures is a consequence of changes in electron temperatures, which are just in this range. For example, the high vibrational temperatures (>6000 K) in the time interval, where the plasma is detached (3.2–3.8 s) indicates low electron temperatures of the order 3 eV. The molecular bands themselves thus offer a convenient criterion for the electron temperatures, which have to be used for analysis of the molecular fluxes. At T_{vib} of 7500 K or higher, it is only clear that T_e must be below 3 eV and it was set to 2.5 eV in the interpretation of the influxes. Once T_e is higher than 5 eV, the $(S_{eff} + D_{eff})$/XB ratio is nearly constant and therefore the choice of T_e is no longer critical. For T_{vib} < 5000 K the ratio 100 was used.

Results for the hydrogen molecular influxes as a function of time and LOS are shown in Fig. 5. In order to get sufficient intensity, the measured spectra were integrated over time intervals of 0.5 s, thus representing average values for the respective time windows. The fluxes show a pronounced increase during the time of detachment. In the raw signals, this increase is partly masked by the fact that $(S_{eff} + D_{eff})$/XB also increases due to lower electron temperatures. The atomic hydrogen fluxes, as derived from H_β intensities or probe saturation currents, show a very similar behavior with time. A typical ratio of molecular-to-atomic particle fluxes of the order 0.5 was obtained by B2-EIRENE [10,11] calculations simulating a density scan, and therefore, the molecular flux is expected to be between 1–4 × 10^{22} m^{-2} s^{-1} depending on time. As can be seen in Fig. 5, the measured absolute values are only in the range of 1 × 10^{22} m^{-2} s^{-1} decreasing to 2 × 10 ^{21} m^{-2} s^{-1}, which means they are about a factor 5 lower than expected. This discrepancy may still be within the error bars of the method and the measurements, however, a tendency to lower results appears very likely.

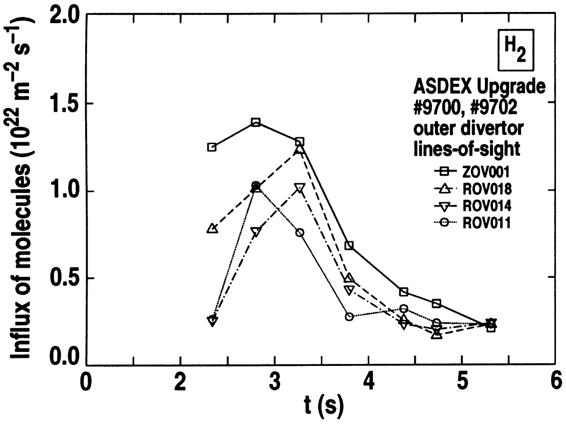

Fig. 5. Measured influx of molecules as a function of time and LOS.

The total intensity of the Fulcher system was also compared directly to B2-EIRENE predictions using the electron impact emission rate coefficient. On the basis of the numerical solution for the molecular densities and electron temperatures, LOS integrated Fulcher intensities were calculated applicable to the present experimental data. The calculated emission is more than 1 order of magnitude (≈50) above the measured values, which is certainly outside the error limits. The present version of B2-EIRENE does not take into account vibrational excitation of the molecules, which, however, will be corrected soon. This means that the ionization and dissociation rate coefficients used in this code are too small by factors of 2–10, depending on temperature, see Fig. 2, and that the predicted molecular densities are too high. Since the emission of the Fulcher bands will be highest in those plasma regions, where the molecular densities are already fairly low due to dissociation processes at lower electron temperatures, it is very likely that this difference in ionization and dissociation rate coefficients can explain the discrepancy to the present experimental results.

As mentioned above, the molecular influx was also determined by using a singlet system of the H_2 molecule (identical plasma parameters). These fluxes show the same dependencies on time and LOS, but are higher than those from the Fulcher system. The discrepancy between the results from the two transitions is known from measurements in low pressure plasmas, where differences between 2 and 10 have been seen depending on electron temperature. Detailed diagnostics of those plasmas demonstrate that hydrogen molecular densities are overestimated by an analysis of the singlet system, while they are underestimated by the Fulcher radiation measurement. The reason is yet unexplained. With respect to measurements of D_2 and the discussed uncertainties of the singlet system, the emission of the Fulcher system is preferred, which also contains information on the ground state vibrational excitation and electron temperature.

4. Summary

The band emission in the Fulcher system of hydrogen and deuterium was investigated in the divertor plasmas of ASDEX Upgrade. A spectroscopic method was introduced for determining molecular fluxes, densities and vibrational population in the ground state. The influx of hydrogen molecules was determined from the population of the upper Fulcher state using the theoretical number of ionization and dissociation events per Fulcher photon $(S_{\mathrm{eff}} + D_{\mathrm{eff}})/XB_{\mathrm{Ful}}$, as calculated by a collisional-radiative model. The Fulcher multi-line spectrum was also analyzed with respect to rotational and vibrational population of the upper state. The influx results were compared with expectations on the basis of the atomic hydrogen fluxes and a typical molecule/atom ratio. Measurement and calculation agree in their time dependence, but the experimental values are somewhat lower. The Fulcher radiation was also compared directly to B2-EIRENE predictions, resulting in a higher discrepancy. In addition, the vibrational population of the ground state was determined from that of the excited state using a method based on Franck–Condon factors. It can be characterized by a T_{vib} between 3000 and 9000 K, inversely correlated with electron temperature. This variation is predicted by the collisional-radiative code and even allows an estimate of T_{e}. Vibrational excitation increases ionization and dissociation rate coefficients. It is therefore very likely that the observed discrepancy in molecular intensity is mainly caused by the omission of vibrational excitation in the present version of B2-EIRENE. The described flux measurements are expected to be accurate above $T_{\mathrm{e}} = 5$ eV, but are more difficult at lower temperatures due to the strong T_{e} dependence of $(S_{\mathrm{eff}} + D_{\mathrm{eff}})/XB_{\mathrm{Ful}}$ in that region. A singlet transition in H_2 was also employed for flux measurements, which gives somewhat higher results, but with higher uncertainties. It is not applicable in deuterium.

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