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On the measurement of molecular particle fluxes in fusion boundary plasmas

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Abstract

This paper describes the determination of the molecular deuterium particle flux Γ_M by means of Fulcher-α-band spectroscopy. As previous investigations have shown [1], the measurement of the molecular flux is essential for an accurate determination of the total deuterium flux released from carbon plasma-facing components. Experiments have been carried out to ascertain the number of deuterium molecules released from a test limiter in the plasma edge of TEXTOR. For different plasma conditions, a molecular flux up to $\Gamma_M \simeq 5 \times 10^{20}\ \mathrm{s}^{-1}$ was measured. Fulcher-α-band spectroscopy is introduced as a straightforward method for the determination of Γ_M. We describe photon flux measurements, a comparison with Eirene calculations, and finally the determination of recycling particle fluxes. The conversion factor D/XB taken from a collisional-radiative model (CRMOL) and relating the number of molecular losses per photon was verified in gas injection experiments.

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1. Introduction

The role of hydrogen and its isotopomers in the plasma edge of Tokamaks is still under discussion [2,3]. In a fusion reactor, the majority of the fuelling gas will enter the plasma via recycling from plasma-facing components such as limiters or divertors. The flux Γ of re-emitted particles is of special interest for a correct interpretation of the recycling process. These particles can be re-emitted both as molecules and atoms depending on the material and its surface conditions. Earlier measurements at graphite limiters in TEXTOR indicated that, under cold surface conditions, the release is dominantly molecular [1].

If molecules are not taken into account, the Balmer-α measurement, a standard method for total hydrogen flux determination, leads to an underestimation of Γ by a factor up to two [4]. Thus, the measurement of Γ_M – the molecular part of Γ – is crucial. Fulcher-α-band spectroscopy allows us to determine Γ_M. In TEXTOR, experiments in D have been performed to investigate the dependence of Γ_M on the plasma parameters and validate the factor D/XB – calculated by a collisional radiative model (CRMOL) – in the range covered.

2. Experimental setup and plasma conditions

The measurements were made in front of a graphite test limiter (0.12 m × 0.08 m, $r = 0.07$ m) positioned at

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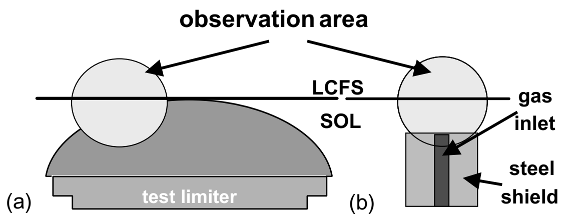

Fig. 1. Observation volumes in front of (a) the test limiter and (b) the gas inlet.

the last closed flux surface (LCFS) at TEXTOR ($R = 1.75$ m, $a = 0.46$ m). The limiter temperature was dependent on the temperature of the actively heated liner (620 K). For calibration purposes, a gas inlet was installed instead of a limiter, 30 mm behind the LCFS. This actively heated effusive nozzle ($T = 620$ K, $d = 8$ mm) consisted of about 300 thin tubes and created a well collimated beam.

A horizontal observation port with a tangential view on either the limiter or the nozzle was used for the spectroscopy [5]. The Fulcher-band was recorded by means of a spectrometer system, which consists of a fiber optic system, a 0.8 m spectrometer in Littrow arrangement and a linear OMA (PARC 3000) detector. The spectrometer is used in second order with a spectral resolution $R = \lambda/\Delta\lambda$ of 13 000, corresponding to a $\Delta\lambda$ of 50 pm. The integration time was routinely set to 0.2 s. The observation volume (Fig. 1) is in the case of the limiter, located at the strike zone, and in the case of the nozzle, in front of the tip.

Six series of discharges were performed with variation of the local electron temperature T_e and density n_e, measured by a helium-beam diagnostic in the midplane; kT_e lay between 33 and 84 eV and the corresponding n_e between 1.3×10^{18} m^{-3} and 15.2×10^{18} m^{-3} at the LCFS during the flat-top phase. The high density discharges were conducted with additional heating (NBI) of about 1.3 MW. The plasma conditions were held constant for six additional discharges to cover the necessary wavelength range of 45 nm with the available spectroscopic system which has just more than 8 nm spectral range.

3. A spectroscopic method for the determination of Γ_M

The main assumption for determination of Γ_M from line emission in high temperature plasmas is the equivalence between photon flux and number of molecular loss events per second. Molecular formation by means of recombination is negligible within this temperature range ($T_e > 10$ eV). The loss events, mainly dissociation and ionisation processes, are characterised by the total decay rate D. Furthermore, if the excitation rate X and the branching ratio B of the transition observed are known, Γ_M can be described by the photon flux ϕ_M and the number of loss events per photon D/XB:

$$\Gamma_M = \frac{4\pi}{h\nu} I_M \frac{D}{XB} = \Phi_M \frac{D}{XB}$$

Neither D nor X are constant, but vary with n_e and T_e. However, Γ_M can be determined by measuring ϕ_M and the local parameters and supplying an appropriate value for D/XB.

3.1. Fulcher-α-band spectroscopy

The Fulcher-band shown in Fig. 2 is the strongest and least disturbed band of D_2 in the visible range [6]. In principle, ϕ_M represents the summation over all line intensities corrected with respect to the line strength, that result from rovibrational transitions between the $3p\,^3\Pi_u$ and the $2s\,^3\Sigma_g^+$ state. An actual summation is not feasible because of the weakness and interferences of some lines. The following procedure describes a simplification, where the total summation is replaced by the summation of one branch only, with the additional help of rotational temperatures as auxiliary quantities for the evaluation of the overall population and accordingly of the total intensity.

The strongest bands are the diagonal ones with equal vibrational number $v = v' = v''$. They are preferred because of the almost identical configuration coordinate of the corresponding electronic states. The matrix of the Franck–Condon factors (FCF) is nearly diagonal. The non-diagonal transitions can be considered by means of appropriate branching ratios [7].

The contribution of one vibrational level is determined by the rotational population within that level. The selection rules for rotational transitions allow three branches: P ($\Delta K = -1$), Q ($\Delta K = 0$) and R ($\Delta K = 1$), where K represents the rotational quantum number. Q belongs to the Π_u^-, P and R belong to the Π_u^+ substate, which is disturbed and thus difficult to use. Fortunately, the sum of the rotational transition probabilities, the so-called Hönl-London factors, for P and R is identical with that for Q. Hence *only* measuring Q and doubling its intensity is sufficient for the determination of the intensity of one vibrational level [5]. The main focus of the ϕ_M determination lies on the correct measurement of the Q-branch intensity of the diagonal transitions. The population of each individual Q-branch is fitted by means of a Boltzmann distribution. This fitting procedure enables us to simulate disturbed lines, and thus the total intensity of a vibrational level can be measured by recording one branch. A summation over all levels leads to the total intensity and to ϕ_M.

3.2. Experimental determination of D/XB

To determine D/XB, calibration experiments using an effusive nozzle have been done. In such D_2 injection

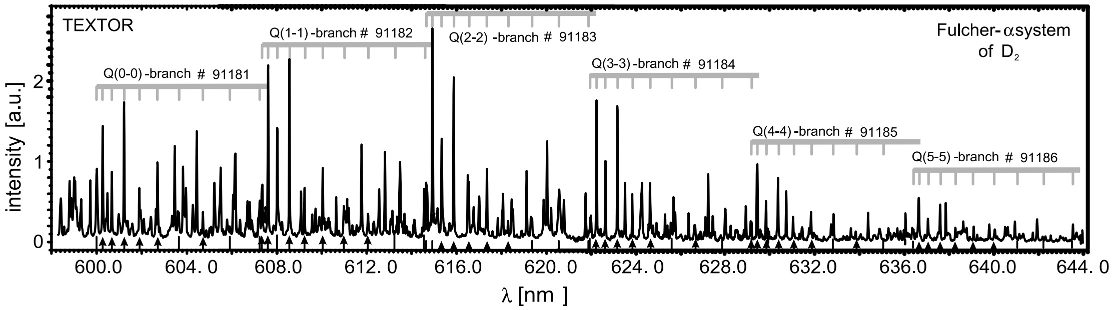

Fig. 2. # 91181-86. The Fulcher-band system of D_2 was observed in front of the gas inlet. The first lines of each Q-branch of the visible diagonal transitions are marked.

experiments, the number of particles and thus Γ_M is known and the corresponding ϕ_M is measured by the method described. The comparison between both quantities results in a value for D/XB for one plasma parameter set.

For an accurate calibration, several critical points have to be considered: (a) The recycling flux has to be excluded from the injected flux. This can be achieved by using a nozzle with minimised surface area far away from other recycling objects as well as by a background subtraction. (b) The injected amount has to be small enough to avoid any disturbances of the plasma and large enough for sufficient intensity. For this purpose, the injected flux has been limited to a low percentage of the usual recycling flux. (c) Finally, the observation volume has to be large enough to detect all photons resulting from the injection.

In series # 91181, 6.5×10^{19} particles were injected into the boundary plasma. Six identical discharges with identical gas injections are necessary to cover the whole wavelength range. The time evolution of ϕ_M follows immediately the injected particle pulse. Fig. 3(a) shows the relative population of the vibrational levels of the $3p\,^3\Pi_u$ state normalised to the $v = 0$ level, obtained by the summation of the rotational line intensities for each vibrational level.

A summation over all intensities and an additional extrapolation to the asymptotic value yields ϕ_M and a D/XB value of 980 ± 245 for $n_e = 0.5 \times 10^{18}$ m^{-3} and $T_e = 50$ eV is obtained. n_e and T_e correspond to the radial location of the maximum emission, 2 cm away from the top of the nozzle, although the measured D/XB represents an average value over the radially extended emission region. The error is determined by uncertainties in the asymptotic extrapolation and the reproducibility of the discharges.

The $3p\,^3\Pi_u$ state is pre-dominantly populated from the $1S\,^1\Sigma_g^+$ ground state [7]. If we assume a thermal distribution for the first vibrational levels in $1S\,^1\Sigma_g^+$, a vibrational distribution in $3p\,^3\Pi_u$ can be calculated via the FCF. Minimisation of the difference between the calculated and measured distribution of the occupancy of the vibrational levels of the $3p\,^3\Pi_u$ state gives T_{vib}, an auxiliary quantity which best represents the vibrational ground state population. In Fig. 3(a) the best-fitted $3p\,^3\Pi_u$ population is shown.

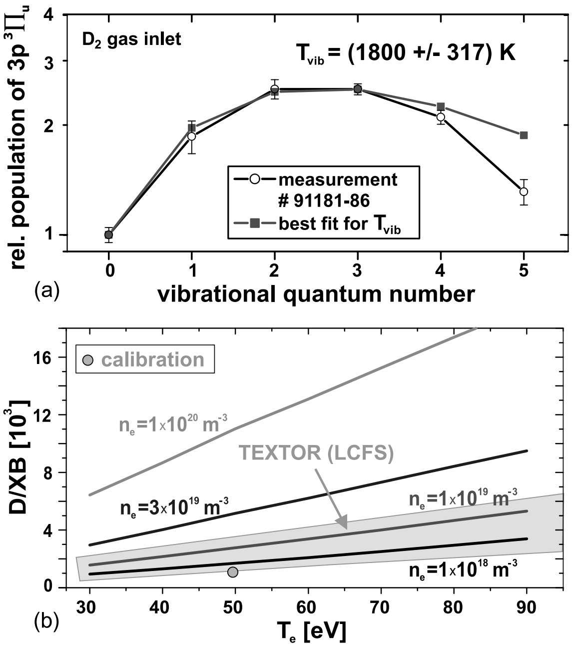

Fig. 3. (a) # 91181-86. The vibrational population of the $3p\,^3\Pi_u$ state for $v' = v'' = 0$–5 and the best fit for T_{vib} in the $1S\,^1\Sigma_g^+$ state for a D_2 injection are shown. (b) CRMOL calculations for the conversion factor D/XB.

3.3. Modelling of D/XB

CRMOL [7] was used to take into account the T_e and n_e dependence of the relevant rate coefficients D and X and thus of D/XB. In addition to dissociation and ionisation, other loss processes like dissociative attachment were included in the calculations. CRMOL solves the coupled rate equations and provides the rate coefficients for the loss and excitation processes as a function of n_e and T_e. Fig. 3(b) displays the variation of D/XB between 500 and 7000 in the respective TEXTOR boundary layer parameter range.

A comparison with the calibration data suggests that D/XB varies between 750 and 1500 over the observed area. CRMOL calculates a value of 1040 for the region of maximum emission at $r = 47$ cm. Thus, the injection experiment confirms the model in the low n_e regime. The calculations of D/XB, verified in this way, were used for further recycling experiments and provide the missing information for Γ_M.

4. Experimental results on recycling fluxes and discussion

Fig. 4(a) shows the incremental increase of ϕ obtained by summation over the contributions of each vibrational level. The data is already corrected to include the effect of the branching ratios, which grow with increasing v. The main contribution results from the first six levels, whereas for higher levels the contribution is smaller owing to pre-dissociation. The asymptotic value represents the total flux ϕ_M from the Fulcher-band transition that we use below. The small difference between the measured value for ϕ_M and the extrapolated one is depicted in Fig. 4(b). The ratio of the population of the first branch to the sum of all branches, which is proportional to the ratio of the corresponding photon fluxes, is shown as a function of T_{vib}.

A simulation of ϕ_M for the six discharge types was made by means of Eirene [8]. Using the measured radial profiles for n_e and T_e as well as an integrated collisional-radiative model based on CRMOL, Eirene simulates the molecular behaviour for the test limiter geometry. ϕ_M is thereby poloidally integrated over the whole limiter and over the same observation volume as the measurement. Fig. 4(c) shows the increase of the measured ϕ_M with n_e in comparison with the modelling of the corresponding cases. For higher values of n_e, a discrepancy between modelling and measurement is noticeable, which might be caused by minor deviations in the determination of local edge parameter profiles.

Multiplication of ϕ_M with the appropriate value of D/XB (Fig. 3(b)) finally leads to Γ_M. Fig. 4(d) displays Γ_M for the same discharge series. The molecular flux has thus been determined as an absolute number of particles. Γ_M rises from 0.2×10^{20} s^{-1} for the low density case to 4.4×10^{20} s^{-1} in the auxiliary heated high density case.

Finally the contribution of Γ_M to the totally released deuterium particle flux Γ is of main interest. The total flux can be described as $\Gamma = \Gamma_A + 2\Gamma_M$ whereas Γ_A represent the pure atomic flux. Previous investigation in discharges with constant plasma conditions – $n_e = 5.2 \times 10^{18}$ m^{-3}, $T_e = 42$ eV at the LCFS – have shown that for graphite as a plasma-facing component the composition of the released species changes with the surface temperature above a threshold of 1100 K [4,5].

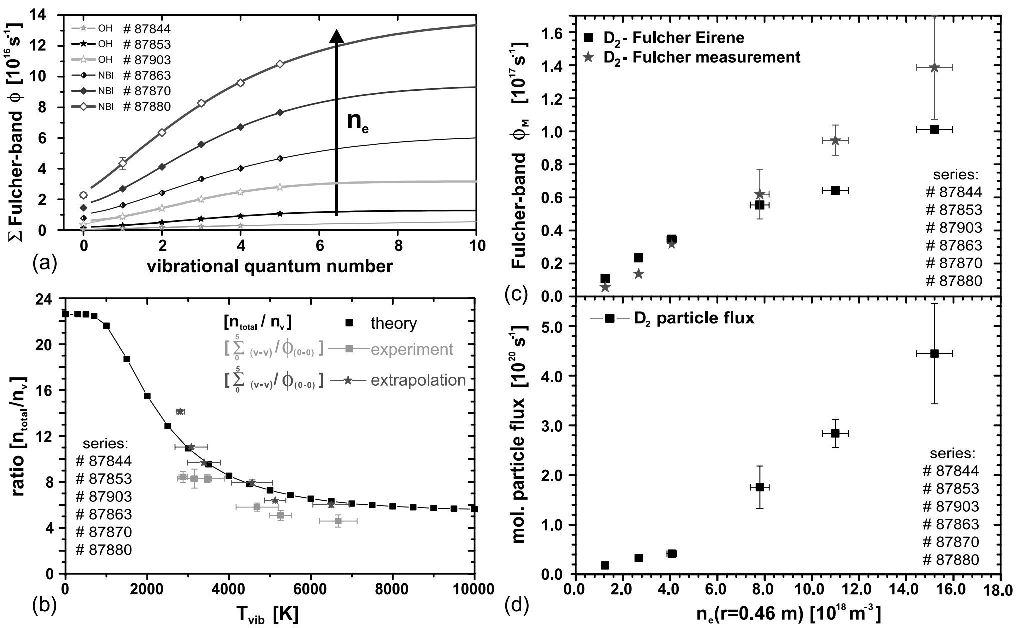

Fig. 4. # 87844-87880. (a) Summation of the photon flux. (b) Ratio of the population of the first vibrational state to the intensity of all states. (c) ϕ_M as a function of n_e. (d) Γ_M determined from ϕ_M using D/XB.

Below this surface temperature the ratio of molecules to atoms is constant and the release predominately molecular. About 90% of the deuterium starts as molecules. Therefore $2\Gamma_M$ represents nearly 90% of Γ [5]. The remaining part of Γ can be described by reflected particles, which start directly as atoms from the surface.

5. Summary and conclusion

Fulcher-α-band spectroscopy has been presented as a method for the determination of the photon flux ϕ_M. The method demonstrates that ϕ_M itself can be determined by the *sole* knowledge of the rotational population of the Q-branches of the diagonal transitions, that is by the intensity of these Q-branches. The molecular flux Γ_M is ultimately deduced from ϕ_M by taking into account the conversion factor D/XB, which was not only taken from a CRMOL, but was also verified in gas injection experiments at TEXTOR.

Significantly high molecular particle fluxes in the order of several 10^{20} s^{-1} were measured in front of a graphite test limiter, located at the LCFS at TEXTOR. The measured increase of these fluxes with the local plasma edge parameters was verified by means of the Monte-Carlo code Eirene. Thus we conclude that Fulcher-α-band spectroscopy in combination with CRMOL represents a straightforward method for the determination of Γ_M.

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