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Vibrational population of the ground state of H_2 and D_2 in the divertor of ASDEX Upgrade

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Abstract

Molecular hydrogen isotopes in the divertor region of fusion experiments may affect the divertor plasma via dissociation, ionization and recombination processes [1]. These processes depend on the vibrational population of the ground state of the molecules. The vibrational populations of D_2 and H_2 were investigated simultaneously at similar divertor plasma conditions, i.e., degree of detachment. The spectroscopic method [2] used, yields vibrational temperatures of 4000–6000 K in the outer divertor, depending on plasma parameters. The isotopes show tendencies, known from laboratory experiments [2], especially similar vibrational ground state populations up to $v = 4$. As previously shown for pure hydrogen discharges [3], the interpretation of experimental data and plasma edge simulations (B2-EIRENE) needs a collisional-radiative (CR) model for H_2. With respect to isotope investigations the measurements and parameter studies show that the transfer of the CR model to D_2 needs an implementation of complete data sets, i.e., rate coefficients, or at least reliable scaling of the input data given.

Keywords: Divertor detachment; Divertor spectroscopy; ASDEX-Upgrade; Collisional-radiative model; Hydrogen molecules

1. Introduction

The presence of hydrogen or deuterium molecules in the boundary layer of fusion plasmas offers several investigation features. As the molecules modify the plasma performance via processes like dissociation, ionization or recombination, they have to be taken into account, when describing the energy balance and the detachment regime of fusion plasmas with a divertor. For general discussion of these features see [1]. The vibrational population of the molecular electronic ground state $X\,^1\Sigma_g^+$ plays a major role in these considerations due to a resonant character of some of the rate coefficients. The population is produced mainly by interaction with the plasma, i.e., electron collision processes.

Using the spectroscopic diagnostic method discussed in detail in [2,3], the relative ground state population can be determined sensitively for vibrational levels up to $v = 4$. For the levels $v > 4$, it has to be supplemented by a CR model for molecular hydrogen [4,5]. The diagnostics is based on the analysis of the diagonal Fulcher bands ($d\,^3\Pi_u \rightarrow a\,^3\Sigma_g^+$) and the Franck–Condon principle of excitation. This can be justified, due to the fact that at electron densities of some 10^{19} m^{-3}, being typical for divertor conditions, the electronically excited states are mainly populated by electron collision excitation from the ground state. Therefore, cascade processes from higher electronic states play a minor role. By attributing a vibrational temperature T_{vib} to the electronic ground state and assuming population via the Franck–Condon principle, the upper Fulcher state vibrational distribution measured can be fitted with $T_{vib}(X\,^1\Sigma_g^+)$ as a parameter. For these calculations, Franck–Condon factors, branching ratios, effective lifetimes and vibrationally resolved rate coefficients are used. The method was demonstrated as applicable to both H_2 and D_2 in

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low temperature plasmas [2]. It has also been applied to hydrogen discharges at ASDEX Upgrade [3] and used by the spectroscopy group of TEXTOR [6]. In ASDEX Upgrade it was demonstrated for pure hydrogen L-mode discharges that the vibrational distribution varies with plasma conditions. In the attached plasma regime the population corresponds to low $T_{vib}(X^1\Sigma_g^+)$ of 3000 ± 500 K, but T_{vib} increases in the detached regime up to 9000 ± 500 K. Furthermore, it turned out that the molecular vibrational levels have to be taken into account as metastable particles in plasma edge models, i.e., B2-EIRENE [3].

In order to improve the method and to get a better understanding of the underlying physics, these investigations had to be extended. Here this was done not only for hydrogen but also for deuterium as isotope behaviour is of high interest for divertor physics.

Previous measurements at ASDEX Upgrade took into account two diagonal Fulcher bands of hydrogen [3]. The derived $T_{vib}(X^1\Sigma_g^+)$ are more reliable, the more transitions of the Fulcher system are measured. This, however, is problematic, as the first four Fulcher diagonal bands of hydrogen cover a wavelength region of more than 40 nm. The need for sufficient spectral resolution, to identify the molecular lines, limits the detectable wavelength region per one plasma discharge. In order to measure more transitions for hydrogen and to measure deuterium, an experimental campaign was carried out at ASDEX Upgrade, including four identical deuterium plasma discharges with local hydrogen injections through one divertor valve. The experimental setup and measured ground state vibrational populations, as well as rotational temperatures of the upper Fulcher state, are presented in Section 2.

For investigation and interpretation of molecule isotope behaviour in divertor plasmas, a transfer of the plasma codes, especially the CR model, from hydrogen to deuterium is required. This need is based on different energy scales of the vibrational (and rotational) levels of the isotopes which leads to significant differences in rate coefficients for excitation, dissociation, ionization, etc. First approaches to introduce deuterium in the CR model are described in Section 3 followed by a conclusion in Section 4.

2. Experimental results on the ground state vibrational population of H_2 and D_2

One major point of this section is the result for the ground state distribution of D_2. The other major point concerns the improvement of the spectroscopic method for H_2. Additionally, the rotational temperatures of the upper Fulcher state are presented as these are derived from the same spectra. The measurements were carried out in a series of special designed deuterium discharges at ASDEX Upgrade with density as well as neutral beam injection (NBI) power ramps. During the discharges the NBI power was increased stepwise up to nearly 8 MW, the line averaged midplane electron density reached 6×10^{19} m^{-3} and the neutral density in the divertor increased up to 8×10^{20} m^{-3}. Injections of molecular hydrogen in the overall deuterium plasma, through one (outer) divertor valve at two time intervals, enabled synchronous measurements of D_2 and H_2. The small amount of injected hydrogen did not change the overall plasma performance, e.g., the degree of detachment, in the divertor. The hydrogen puff may have cooled the plasma locally in a volume of approximately 1 cm^3 near the valve, due to a local increase of neutral density and therefore a stronger recycling. The Fulcher emission was detected using a 1 m spectrometer and a CCD camera providing a spectral resolution of 0.05 nm. Thus the wavelength region 600–630 nm was covered by the four identical discharges; this being equivalent to the diagonal bands up to $v' = v'' = 2$ (2–2) for hydrogen and up to 3–3 for deuterium. Especially, the lines Q1–Q6 of the Q-branches were analysed. During the injections, hydrogen radiation was observed via three poloidal lines-of-sights (LOS), labeled ZOV001-003 (shown in [1]). The undisturbed deuterium radiation was measured by using ZON003 (equal to ZOV003, but located in another section of the torus).

Rotational and vibrational populations were determined at three time intervals. Two of them ($t1 = 2.1$ to 2.6 s; $t3 = 4.3$ to 4.8 s) correspond to the hydrogen injection, $t1$ referring to low power input and densities and $t3$ referring to high power and densities. At the time interval $t2 = 3.0$ to 4.0 s these parameters range in between. As can be seen in Fig. 1, the rotational temperatures T_{rot}, as derived from 'Boltzmann Plots' for Q1–Q6, differ significantly for the various diagonal transitions of the upper Fulcher state $d\,^3\Pi_u$. At $t1$, the

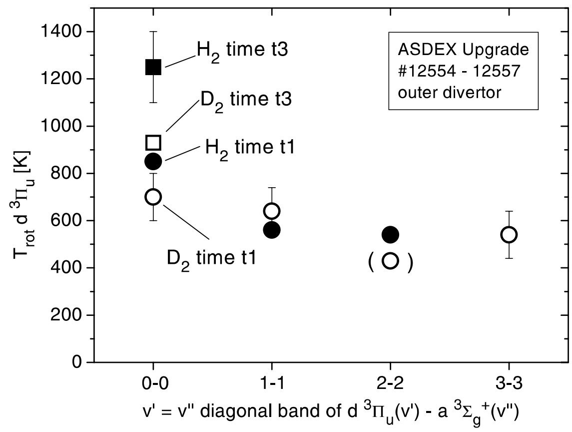

Fig. 1. Rotational temperatures of the upper Fulcher state for D_2 and H_2, derived from different diagonal transitions.

$v' = v'' = 0$ (0–0) band gives 800–900 K for hydrogen, whereas the 1–1 and 2–2 bands give 500–600 K. This drop in T_{rot} confirms former measurements at ASDEX Upgrade and was also found to a lower degree in laboratory plasmas. Tendencies are similar for deuterium. However, the Q-lines of 2–2 deviate from a Boltzmann distribution. T_{rot} drops from 700 to 600 K for 0–0 and 1–1, respectively, to 430 K in the 2–2 band, and increases again in the 3–3 band. As these perturbations were neither observed for hydrogen nor for laboratory plasmas, they are subjects for future investigations. At $t3$, hydrogen emission was only observed for the 0–0 band because of lower expansion of the injected H_2. T_{rot} from this transition was found to be between 1100 and 1400 K. The rotational temperature at $t3$ also increases for deuterium (930 K). This increase for both isotopes may be evidence for heavy particle collisions at higher neutral densities.

Regarding the vibrational populations, good agreement of measured and fitted upper Fulcher state vibrational distributions was found for both hydrogen and deuterium. As explained in Section 1 and described in detail in [2,3], for the calculation of the upper state vibrational population, $T_{vib}(X^1\Sigma_g^+)$ serves as a fit parameter. Figs. 2 and 3 illustrate the fits and the attributed vibrational temperatures of the ground state $T_{vib}(X^1\Sigma_g^+)$. Supplementary to previous measurements [3], the $d^3\Pi_u$ ($v' = 2$) population of H_2 agrees just as good as $v' = 1$ with the fitted population, confirming the underlying method. Discrepancies for $d^3\Pi_u$ ($v' = 2$) for deuterium, are due to the discussed deviations in the 2–2 transition, whereas $v' = 0$, 1 and 3 are fitted well. The measurements for hydrogen result in $T_{vib}(X^1\Sigma_g^+) =$ 5000–6000 K at $t1$ for the different LOS, error bars being 500 K. In deuterium, $T_{vib}(X^1\Sigma_g^+)$ are 4000, 5000 and 6000 K at $t1$, $t2$ and $t3$, respectively. Due to the different vibrational energy scale of the isotopes, equal populations are characterized by different temperatures. A relative population of 65% in the vibrational ground state $v = 0$ corresponds to a temperature of 4000 K for deuterium and 5500 K for hydrogen. The $T_{vib}(X^1\Sigma_g^+)$ derived from the simultaneous measurements at time $t1$ confirm results from laboratory plasmas, i.e., vibrational levels of hydrogen and deuterium up to $v = 4$ are similarly populated at comparable plasma conditions [2].

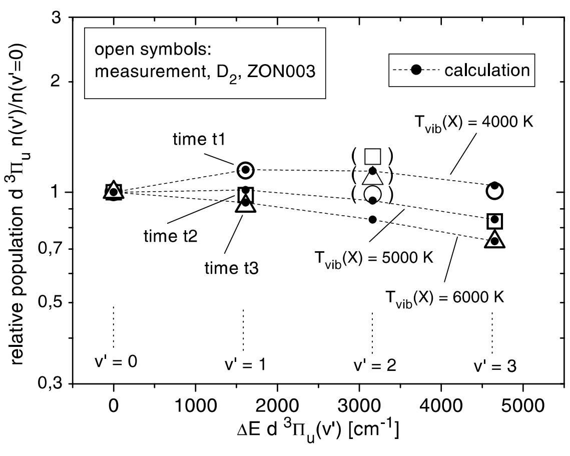

Fig. 2. Vibrational temperatures of the ground state of D_2, measured in the outer divertor at three time intervals of the series #12554–12557.

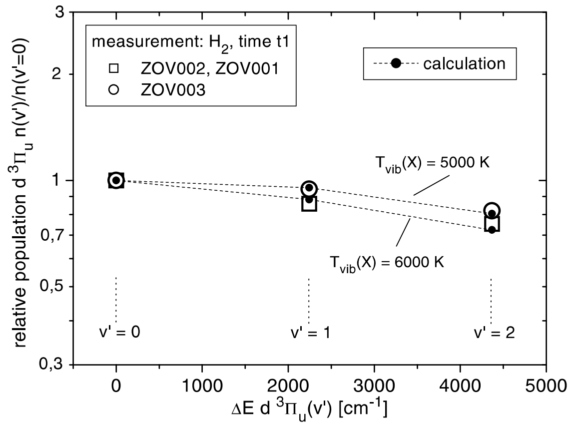

Fig. 3. Vibrational temperatures of the ground state of H_2, measured in the outer divertor for the series #12554–12557.

The increase in $T_{vib}(X^1\Sigma_g^+)$ of D_2 with time, i.e., plasma performance, can be analysed by applying the CR model for hydrogen in which deuterium data has to be implemented as discussed in the following section.

3. Implementation of D_2 in the collisional-radiative (CR) model for H_2

Supplementary to the experimental investigations, the behaviour of hydrogen and deuterium was tested with respect to an implementation of the species in plasma edge codes. Until now, the current CR model for H_2 has been used to calculate effective rate coefficients for processes depending on the molecular vibrational population.

While H and D atoms can be treated equally in the CR model, the isotopic energy shift of the molecular vibrational levels causes differences in rate coefficients which depend on the vibrational population [7]. It had to be tested how the model ought to be modified in order to provide reliable results for deuterium. Currently, five reaction channels depending on the vibrational distribution in the ground state are included in the model:

$$H_2(v) + e^- \rightarrow H_2^- \rightarrow H_2(w > v) + e^- \quad (1)$$

electron excitation

$$H_2(v) + e^- \rightarrow H_2(b) + e^- \rightarrow H + H + e^- \quad \text{dissociation} \tag{2}$$

$$H_2(v) + H^+ \rightarrow H_2^+ + H \quad \text{ion conversion} \tag{3}$$

$$H_2(v) + e^- \rightarrow H_2^- \rightarrow H^- + H \quad \text{dissociative attachment} \tag{4}$$

$$H_2(v) + e^- \rightarrow H_2(B, C) + e^- \rightarrow H_2(w) + e^- \quad \text{electron excitation, radiative decay} \tag{5}$$

Whereas (1) is a populating process, (2)–(4) are depopulating. Process (5) provides redistribution, repopulating preferably higher v levels of the ground state. As a first step towards implementation of D_2, the vibrational level energies were corrected in the model. Taking a closer look at (1)–(5), however, this exchange cannot be assumed to be sufficient. By comparing literature data (e.g. the compilation given in [7]), more or less pronounced differences are found for the isotopes, regarding the discussed channels. Especially, the ion conversion and the dissociative attachment are resonant for energies matching $v = 4$ in hydrogen, but $v = 6$ in deuterium [7]. Therefore, as a second step, these differences were introduced in the CR model for the depopulating channels (2)–(5) by scaling the hydrogen data currently included. The effects of these two steps were tested by calculating vibrational populations depending on electron temperature. Regarding electron density, no dependence was found. In Figs. 4 and 5 the calculated populations are displayed for electron temperatures, 1, 4 and 10 eV, respectively. First of all, the attribution of a vibrational temperature to the first five vibrational levels turns out to be a reasonable assumption. This confirms the spectroscopic method described. Furthermore, for $T_e = 4$ and 10 eV, deviations towards increased population of higher v levels appear, compared with a temperature like curve. The increase is due to the repopulation of the higher v levels by reaction (5). It turns out that step one (energy correction) seemingly increases the ground state vibrational population of deuterium compared with hydrogen. Activation of the scaled rate coefficients counteracts these effects for higher T_e. This effect is not observed for 1 eV, since the different threshold energies of the isotopes for the populating reaction (1) are more important at low electron energies.

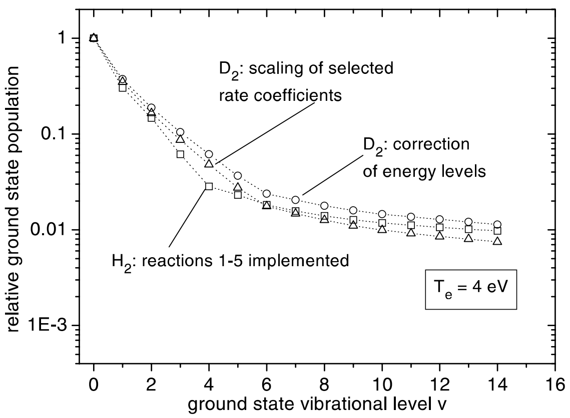

Fig. 4. Relative vibrational population of the ground state of H_2 and D_2, calculated for $T_e = 4$ eV by a modified CR model for H_2 and H.

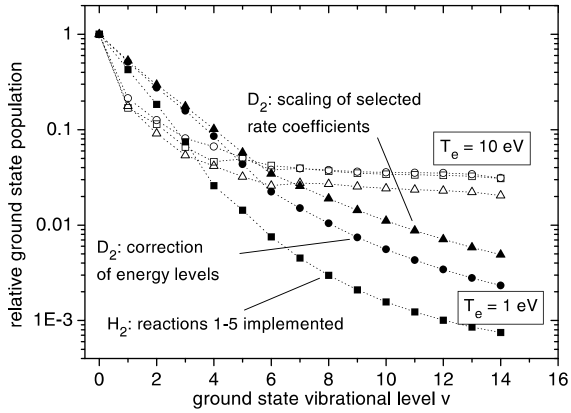

Fig. 5. Relative vibrational population of the ground state of H_2 and D_2, calculated for $T_e = 1$ and 10 eV by a modified CR model for H_2 and H.

On this basis, the vibrational populations measured were used to determine T_e in the observed region of the outer divertor (more detail in [8]). This led to $T_e = 3$ to 4 eV and $T_e = 5$ eV for hydrogen and deuterium, respectively, as derived from the simultaneous measurements at $t1$. The difference in T_e may be due to the rather rough scaling for deuterium, local plasma cooling during the hydrogen puff or even to different initial vibrational populations of the molecules at the wall/valve. One has to bear in mind that this combination of measured vibrational population and CR model provides a T_e-diagnostics for regions near the walls where the molecules radiate. Therefore, the absolute values of the derived temperatures are not expected to agree with other ASDEX Upgrade T_e-diagnostics. The measured increase in $T_{vib}(X\,^1\Sigma_g^+)$ of deuterium with increasing power and densities, results in 5, 3 and 2 eV for $t1$, $t2$ and $t3$, respectively. This decrease in T_e is confirmed by Langmuir probe data.

For the future, the data basis has to be extended generally and available rate coefficients or cross-sections for D_2 have to be included directly. Furthermore, the model should also be transferred to the HD or DT isotope. Under the experimental conditions presented, where hydrogen was injected in deuterium, HD may be formed but its emission was not observed. Regarding the vibrational physics discussed so far, heteronuclear molecules are expected to show differences, since their vibrational levels can decay directly by radiation. Apart from the experimental problems, e.g., overlapping of H_2, D_2 and HD spectra, data base is scarce. Therefore, the development of the approaches introduced, will provide more information concerning scaling laws for isotopes, important for fusion plasmas.

4. Conclusions

The spectroscopic diagnostics for the relative ground state vibrational population was established for D_2 in the divertor plasma of ASDEX Upgrade. Concerning H_2, the inclusion of the 2–2 vibrational Fulcher transition into the measurements proved to be a useful extention of the diagnostic tool, as used up to now at ASDEX Upgrade. Simultaneous measurements of the isotopes revealed similar relative vibrational populations of the ground state. A variation of $T_{\mathrm{vib}}(\mathrm{X}\,^1\Sigma_g^+)$ of D_2 in the outer divertor during the power and density ramp was found. First attempts were made to transfer a CR model for molecular hydrogen to deuterium. It was discussed that apart from simple scaling of given hydrogen rate coefficients, complete sets of isotope data have to be used in order to prepare the model for future implementation in plasma edge modelling.

References

[1] U. Fantz, D. Reiter, B. Heger, D. Coster, Hydrogen molecules in the divertor of ASDEX Upgrade, these Proceedings.
[2] U. Fantz, B. Heger, Plasma Phys. Control Fusion 40 (1998) 2023.
[3] U. Fantz, K. Behringer, J. Gafert, D. Coster, ASDEX Upgrade team, J. Nucl. Mater. 266–269 (1999) 490.
[4] K. Sawada, T. Fujimoto, J. Appl. Phys. 78 (1995) 2913.
[5] P.T. Greenland, D. Reiter, Report JUEL-3258, 1996.
[6] A. Pospieszczyk et al., J. Nucl. Mater. 266–269 (1999) 138.
[7] Celiberto, A. Laricchiuta, M. Capitelli, R.K. Janev, J. Wadhera, D.E. Atems, IAEA INDC(NDS)-397 (1999).
[8] U. Fantz, B. Heger, D. Wünderlich, submitted.