
Molecular Deuterium Behaviour in Tungsten Divertor on JET
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ABSTRACT
Molecular spectroscopy was used to observe molecular deuterium at the outer strike point of the new bulk tungsten JET divertor. The rotational and vibrational populations of the deuterium molecules in the ground state were determined from the deuterium Q-branches of Fulcher-α band emission \( (d^3\Pi_u^- \rightarrow a^3\Sigma_g^+) \) in the 600–640nm spectral range. For L-mode plasmas in the low recycling regime the molecular emission maximum is close to the strike point. The spatial profile of the emission was strongly modified during plasma detachment in both L- and H-mode plasmas. The rotational temperature of excited molecules reached 2760 K in L-mode. The vibrational population has a peculiarity: a remarkably high population of the \( d^3\Pi_u^- (v = 0) \) vibrational level indicating a non-Boltzmann vibrational distribution of \( D_2 \) in tungsten environment.

1. INTRODUCTION
Recycling in the divertor plays an important role for plasma fueling in tokamaks. Neutral particles are formed on the target surface due to neutralization of the impinging plasma ions. The neutrals are then reemitted from the surface and ionized in the plasma. Depending on the material and the surface temperature, deuterium can be reemitted as an atom or as a molecule. In contrast to an atom, a molecule has a longer destruction chain in the plasma due to the additional dissociation process. The source position of the charged particles inside the plasma strongly depends on the type of reemitted particles. In addition, the presence of vibrationally excited deuterium molecules can increase the recombination rate in cold plasmas and have vital impact on the divertor operation. The previously performed JET measurements with the full carbon divertor [1] have confirmed that deuterium release from the divertor walls dominates in the form of molecules as in TEXTOR [2]: molecules contribute between 70% and 90% to the total deuterium influx. Thus, for a correct calculation of the atom fluxes a knowledge of the molecular contribution is needed, otherwise the deuterium influx will be strongly underestimated. Thereby, the atomic and molecular deuterium influx is in the ionizing regime representative for the recycling flux or equivalent the impinging ion flux. In the tungsten environment more ion reflections are expected which should reduce the re-emission of the molecular deuterium and increase the amount of the fast deuterium atoms.

2. SPECTRAL MEASUREMENTS
The upgraded vertical viewing high resolution spectrometer system KT3B [3] was used to measure Fulcher-α band emission \( (d^3\Pi_u^- \rightarrow a^3\Sigma_g^+) \) in the 600–640nm spectral range from the divertor. The Acton 0.75-m imaging Czerny-Turner spectrometer with entrance slit of 20µm is equipped with EMCCD digital camera. The camera sensor provides 1024 pixels with size of 13µm for spectral and 22 tracks for spatial resolution across the horizontal target plate. The central axes of the spectrometer viewing chords are shown on Fig.1. With the 1200l/mm grating, the dispersion of the spectrometer at 610nm is about of 0.0128nm per pixel. All spectra were recorded with an exposure time of 40 ms starting from the beginning of the plasma pulse at 40 s. At present time
only Q-branches of Fulcher-α band emission \((d^3\Pi_u^- \rightarrow a^3\Sigma_g^+)\) are suitable for data analysis. For the measurement of diagonal transition Q(0-0), Q(1-1), Q(2-2) and Q(3-3), the central wavelength of the spectrometer was changed consecutively to 604.5nm, 614.5nm and 624.5nm in the series of reproducible plasma discharges.

3. EXPERIMENTAL RESULTS AND DISCUSSION

The combined spectrum measured during L-mode plasma pulses is shown together with Q-branches line identifications on Fig.2. The spectrum was measured on the optical chord passing through the strike point during 14.98s - 22.9 s at the flat top of L-mode plasma discharges (\(B_t = 2.4T, I_p = 2.0MA, n_e dl (core) \sim 7.9\times10^{19} m^{-2}, T_e (core) \sim 1.5keV, P_{rad} \sim 1.0MW\)). The plasma was additionally heated with 1.0MW NBI and 0.5MW ICRH. The outer strike point was placed on a metallic row of the divertor horizontal target plate consisting of stacks of solid tungsten lamellae [4]. For the plasma fueling, deuterium gas was puffed trough divertor base outer ring (GIM9 on Fig.2) with a rate of about \(6\times10^{21} D/s\). The closest gas injection hole is several centimeters away both poloidal and toroidal directions and is not directly seen by KT3B spectrometer system.

The rotational population of the \(d^3\Pi_u\) levels with vibrational quantum number \(v=0, v=1, v=2\) and \(v=3\) were derived in a standard way [5, 6] from Boltzmann plots of the intensities of the rotational lines normalized to corresponding transition probabilities and degeneration factors versus rotational energy difference with respect to rotational level with rotational quantum number \(N=1\), as shown in Fig.3. The Q(0-0) rotational lines up to \(N=17\) can be resolved. For the fitting, only undisturbed lines were used. One can see that the \(d^3\Pi_u, v=0\) population can be well fitted with the rotational temperature about 2760 K. For the levels with \(v=1, v=2\) and \(v=3\) the rotational temperatures were almost two times lower, respectively 1470 K, 1290 K and 1290 K. These temperatures are higher by a factor of about 2 then the rotational temperatures measured in the carbon divertor for similar plasmas [1]. The rotational temperature of the ground state \(X^1\Sigma_g^+\) derived from the temperature of \(d^3\Pi_u, v=0\) using the ratio of the rotational constants for excited and ground vibronic states [7] \(B_d (v=0)/B_X (v=0) \approx 0.5\) is about 5500 K. The vibrational temperature of the ground state \(X^1\Sigma_g^+\) was expected to be about 27000 K as estimated by the empirical linear scaling of ground state vibrational temperature versus \(d^3\Pi_u, v=0\) rotational temperature \(T_{vib}(X^1\Sigma_g^+)[K] = 10.6\cdot T_{rot}(d^3\Pi_u^- v=0) [K] – 4.3\cdot T_s [K]\), where \(T_s\) is the population temperature of the deuterium molecules entering the plasma [8] (vibrational and rotational temperatures are assumed to be identical).

The vibrational population of the \(d^3\Pi_u\) state found with help of the measured rotational temperatures is shown on Fig. 4. This population usually is non-Boltzmann [2, 5, 6] due to strong impact of the direct excitation from the ground state \(X^1\Sigma_g^+\) and defined mainly by Frank-Condon factors of \(X^1\Sigma_g^+ \rightarrow d^3\Pi_u\) transition and vibrational population of the ground state. In the JET carbon divertor, the observed \(d^3\Pi_u\) vibrational population at the strike point can be well fitted by Boltzmann distribution with vibrational temperatures in the range 4000–5500 K and above mention scaling of vibrational-rotational temperatures coupling was validated. One can see on Fig.4 that the vibrational
level with $v=0$ is strongly populated and such a shape of the vibrational population could not be described with a Boltzmann distribution on the ground state with excitation by plasma electrons in coronal approximation. This could point to a non-Boltzmann vibrational population of the ground state. The rough estimations indicates the possibly strong (more than a factor 10) overpopulation of the ground states vibrational levels with $v = 1$, $v = 2$ and $v = 3$ with respect to the Boltzmann distribution with $T_{\text{vib}}(X^1\Sigma_g^+) = 27000$K. On the other hand, the observed vibrational population of the excited state $d^3\Pi_u$ could be also well described as a sum of 84% Boltzmann distribution with $T_{\text{vib}} = 2760$K and 16% non-Boltzmann due to excitation from the ground state having $T_{\text{vib}} = 2760$K, both equal to the measured $T_{\text{rot}}(d^3\Pi_u^- v = 0)$. If the latter is true, this could indicate a rovibrational relaxation so strong that the levels almost reach the Local Thermo-dynamical Equilibrium (LTE). The reason for such a population distribution is not clear yet and experimental data analysis is still under way.

The total intensity of the Q(0-0) branch has a maximum close to the strike point for L-mode plasma as seen on Fig.5. The plasma continuum radiation measured at wavelength 611 nm has a maximum at the radial position of the Q(0-0) branch intensity, as shown on Fig.6. The rotational temperature also increases toward the strike point but at the strike point itself, the temperature drops by about 600K.

In H-mode density limit Pulse No: 81933 ($B_t = 2.9$T, $I_p = 2.0$MA, $n_e \cdot d_{ll} \sim 2.0 \times 10^{20}$ m$^{-2}$, $T_e \sim 2.0$keV, $P_{\text{rad}} \sim 4.5$MW, $P_{\text{NBI}} = 10.5$MW, gas fuelling: multiple injection in the divertor (GIM9, GIM11 and GIM12) with maximum puff rate $2.2 \times 10^{23}$ D/s, magnetic configuration similar to Pulse No: 81271) [9], both the temperature and the Q(0-0) branch intensity have a maximum at the edge of the bulk tungsten tile ($R = 2.82$m) and decrease toward the strike point, as can be seen in Fig.7. The minimum of the molecular deuterium emission at the strike point is due to an increase of ionizations per photon with the electron density for the Fulcher-$\alpha$ band emission and an increase of the reflection cross-section of deuterons with a decrease of the electron temperature. The divertor electron density in H-mode density limit plasma discharge was much higher than in L-mode plasma. Both the plasma continuum and Paschen/Balmer line series of atomic deuterium show a clear signature of plasma recombination at the strike point.

The measurements in the limiter tokamak TEXTOR [2], divertor tokamak D-IIID and liner plasma device PISCES [10] demonstrate the linear dependence of $T_{\text{rot}}(d^3\Pi_u^- v = 0)$ versus the plasma density with a slope of about $3 \times 10^{-17}$ K/m$^3$ and an offset of 400 - 500 K. Therefore, the rotational temperature is expected to increase with plasma density. The reduction of the rotational temperature at the strike point is related to the same process which is responsible for the local minimum of $T_{\text{rot}}(d^3\Pi_u^- v = 0)$ in L-mode plasma namely the plasma density gradient. A similar behaviour was observed in the carbon divertor: both rotational and vibrational temperatures decrease from the strike point towards the private flux region [1]. One can conclude that the molecules moving in the direction opposite to the plasma density gradient have more probability to be rovibrationally excited before the ionization. Molecules re-emitted from the tungsten surface at the strike point perpendicular to the surface
move in the direction of the plasma density gradient and match the geometry of the measurements performed in [2, 10]. Therefore, the scaling for $T_{\text{rot}}(d^3\Pi_u^{-} v = 0)$ can be used for the evaluation of the local electron density: $T_{\text{rot}}(d^3\Pi_u^{-} v = 0) = 2960$ K corresponds to the electron density of about $8 \times 10^{19}$ m$^{-3}$ at the place of the destruction of the deuterium molecules. The absolute calibration of the divertor imaging spectrometer system for the 600–640nm wavelength range will be done in a near future to determine the molecular deuterium fluxes and the fraction of the molecules in the total influx of the neutral particles.

CONCLUSIONS
Molecular deuterium was measured spectroscopically in the full tungsten divertor of JET. For the attached L-mode plasma, the vibrational population of $d^3\Pi_u$ state of molecules recycled at the strike point demonstrates a peculiarity which could indicate the presence of a non-Boltzmann population of the ground state $X^1\Sigma_g^+$ or the existence of rovibrational relaxation of the ground state as well as excited state $d^3\Pi_u^{-} (v = 0)$. The measured $d^3\Pi_u^{-} (v = 0)$ rotational temperature has a local minimum near the strike point, which could be due to the influence of the plasma density gradients. In comparison with a full carbon divertor, the molecular deuterium in the full tungsten divertor shows higher rotational excitation probably due to higher divertor plasma density and lower electron temperature.

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Figure 1: Viewing chords of KT3 spectrometer and gas injection positions.

Figure 2: Composite spectrum of the Fulcher-α band emission at viewing chord 7, Pulse No’s: 81271, 81273, 81274.

Figure 3: Boltzmann plot for rotational temperatures determination $d^3\Pi_u^0$ level.

Figure 4: Relative vibrational population of $d^3\Pi_u$ state.
Figure 5: Rotational temperature and $Q(0-0)$ branch intensity profiles evolution, L-mode Pulse No: 81271.

Figure 6: Plasma continuum at 611nm, rotational temperature and $Q(0-0)$ branch intensity radial profiles during flat top L-mode Pulse No: 81271.

Figure 7: Rotational temperature and $Q(0-0)$ branch intensity profiles evolution, H-mode density limit Pulse No: 81933.