Spectroscopic observations and analysis of the Fulcher Bands of hydrogen an its isotopologues in divertor region of the ITER-like wall JET tokamak

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Molecular dynamics in the tokamak plasma divertor is currently increasingly included in plasma modeling (e.g. [1, 2] and others). Experimental confirmation of the models can be performed using different methods: comparing the hydrogen and helium results and searching for the "residual" differences, using the calculated intensities of the atomic radiation with and without molecular contributions [3] or directly analyzing the molecular radiation of the hydrogenic molecules [4,5]. For this, the most frequently used are Fulcher-α bands, spreading around the 600 nm spectral region.

These bands are transitions between d ($3p^3\Pi_u$) and a ($2s^3\Sigma^+_g$) levels, and one of the important problems in the analysis of them is that there are very close levels of hydrogen molecule from which transitions overlap in the same spectral region, the most important being g→c transition. The d→a transition is stronger, but this adds complexity to the spectral analysis due to many overlapping lines from different systems.

Recording and analysis of the Fulcher Bands (FB) in JET plasma can be performed by two types of spectrometers – fixed wavelength COS spectrometers observing mostly the limiter regions with one divertor view included (collection angle covers around half the divertor tungsten stack) and the tunable mirror-link spectrometer, observing the outer divertor with 22 parallel lines of sight. The resolution and sensitivity of the tunable spectrometer is better than those of the COSes, but its spectral region is much smaller – to cover the same spectral region it requires 4 spectral settings (4 identical JET pulses), which severely limits its availability for molecular studies. Nevertheless, this spectrometer is crucial for any kind of spatial dependence studies, and in addition the regions with the highest intensity of the Fulcher bands sometimes lie on the verge, or even outside the divertor COS collection angle and can be observed only with the mirror-link spectrometer.

Examples of spectra from three different hydrogen isotopologues are shown in Figure 1, where the main Q branch lines from 0-0, 1-1 and 2-2 vibrational bands are identified. The isotopic effect is visible in the separation of the spectral lines – in hydrogen the separation is largest, in tritium – smallest. The hydrogen spectra are much better resolved and the particular lines needed for analysis may be assumed to be non-blended with any additional lines – in tritium this assumption is much less valid.

An analysis of a spectrum to obtain total intensity of the vibrational transition consists of determining the intensity of the rotational transitions (those which can be identified as non-blended), calculating the rotational temperature for each vibrational transition using the assumption of Boltzmann distribution, and then estimating the total emission coefficient of the vibrational transition from the emission coefficient of the chosen rotational transition using the equation:

$$\frac{I_{J'J''}}{I_{v'v''}} = \frac{S_{J'}}{U_{v'}(T_{rot})} \exp\left(-\frac{E_{J'}}{kT_{rot}}\right)$$

where the primed values are of the upper level of the optical transition, U(T) is the rotational partition function, S_J is the rotational part of the Einstein coefficient and E_J is the rotational energy of the level.

The first studies of the Fulcher band radiation of deuterium in ILW (ITER-like wall) JET divertor were published by Sergienko et al in 2013 [5]. The measured rotational temperatures and vibrational

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population distributions of the d level were much different from the results obtained in the carbon wall machines (also in JET-C [4]) – rotational temperatures in [5] were much higher (up to 4000 K) than previously (~1000 K), and the estimated populations of vibrational levels had a maximum for the lowest (v = 0) vibrational level, not for v = 2.

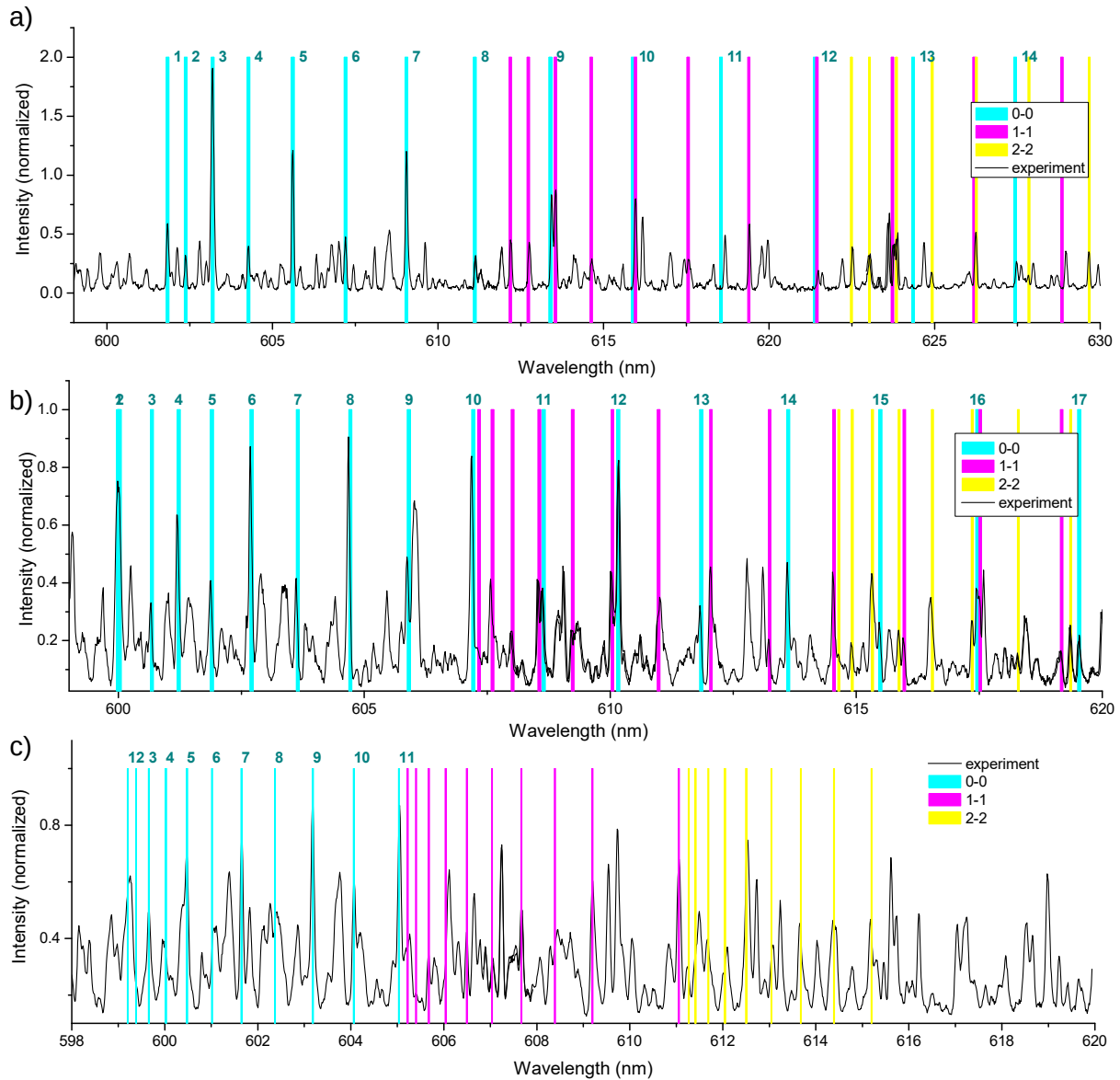**Fig. 1.** Fulcher bands recorded by KT3B with identified Q-branch transitions for the first vibrational levels for a) H_2 molecule, b) D_2, c) T_2. Note, that the hydrogen spectrum has a different wavelength range than other isotopes.

Our results confirm the findings of [5] also for other isotopes – Figure 2a shows the rotational Boltzmann plots for 0-0 and 1-1 transitions in hydrogen, yielding the rotational temperatures of 3700 and 2000 K. Figure 2b shows the spatial distribution of the intensities of 0-0 and 1-1 transitions during the early stage of the #91279 pulse (B = 2.5 T, I = 2.5 MA, auxiliary heating power NBI 1.5 MW, line integrated edge density from 2 to $6 \cdot 10^{19}$ m^{-2}), which is also similar to the reported in [5] – the intensity of the 0-0 transition is higher than 1-1, with relatively constant 2:1 ratio.

The spatial intensity distribution of the 0-0 FB deuterium band over the divertor reported in [5] had two shapes – in one the molecular radiation had a peak close to the strike point (L-mode discharge #81271),

in the other the maximum was much broader and located outside the strike point (H-mode discharge #81933). Our measurements in hydrogen, deuterium and tritium have shown similar intensity distributions (e.g. the one presented in figure 2b). The shape and position of the maximum intensity depends on plasma density; the experiment in deuterium (see figure 3, #94767 and repeats, B = 2.5 T, I = 2.45 MA, auxiliary heating power NBI 1 MW) shows that changing the edge density from 4 to $6 \cdot 10^{19}$ m^{-2} resulted in changing the position of the maximum outwards. The rotational temperatures for the 0-0 band during this pulse are between 2000 and 3000 K, with higher values during the high-density part of the pulse.
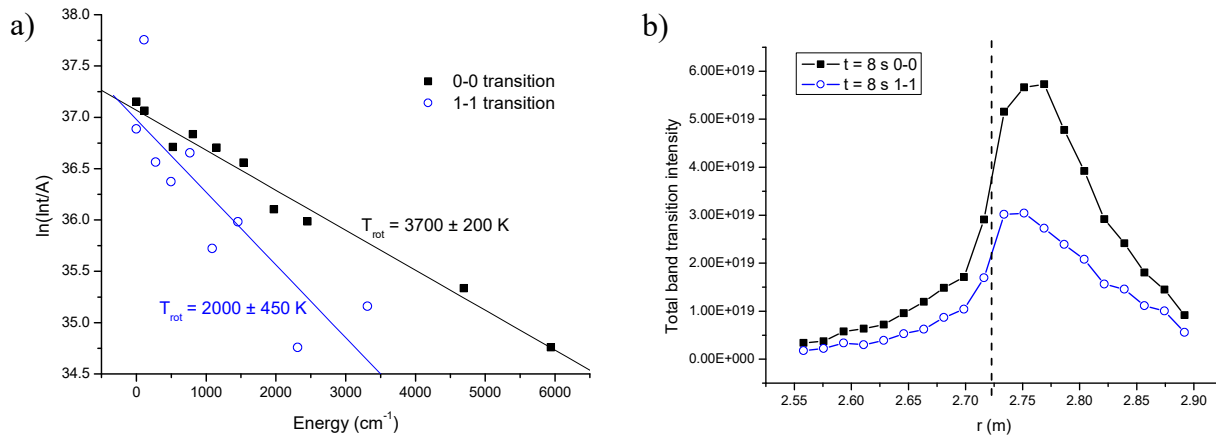

Fig. 2. Results for the H$_2$ pulse #91279 and its repeats: a) Boltzmann plot of the strike point 0-0 and 1-1 rotational population distributions at pulse time 8 s, b) spatial distribution of the band intensities also at t = 8s.
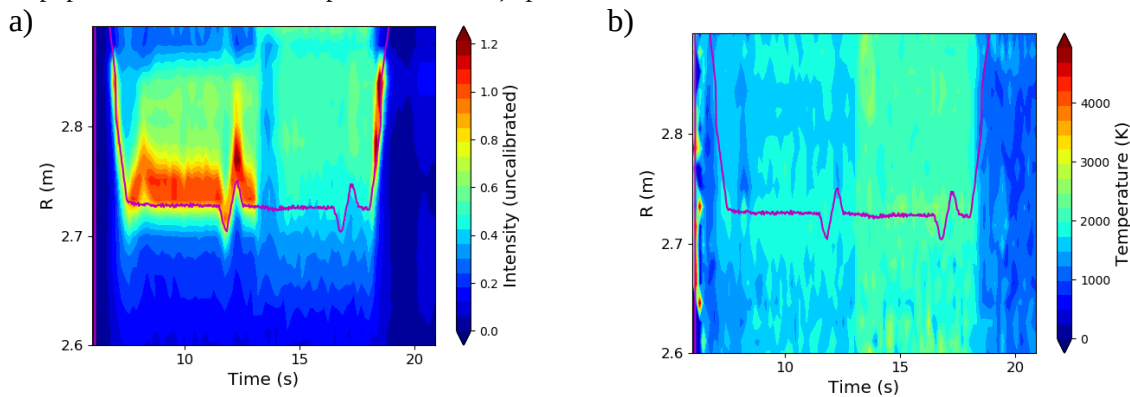

Fig. 3. Evolution of the spatial distributions of 0-0 band a) intensity and b) rotational temperature of pulse #94767 (D$_2$).

Figure 4 shows a comparison between the spatial distribution of the 0-0 transition intensity and the commonly used Balmer D$_\alpha$ line. For low density part the spatial distribution is similar, but for the high density part the D$_\alpha$ intensity also has maximum on the strike point, and its intensity is much higher than for the low-density step, whereas the 0-0 FB transition intensity distribution exhibits broad maximum well outside of the strike point.

We have also attempted to calibrate the intensity of the deuterium 0-0 transition versus the number of particles introduced into the plasma within the spectrometer collection angle (a procedure described in [6]). The camera image of the D$_\alpha$ line intensity for the pulse #95164 and the intensity evolution of the 0-0 band radiation for pulses #95159 (no puff), #95160 (all available D$_2$ in one puff) and #95162 (divided into three puffs) are presented in Figure 5. The introduction of the cold gas considerably lowered the observed rotational 0-0 band temperature, but the temperature recovered when the intensity of the increased radiation reached the maximum.
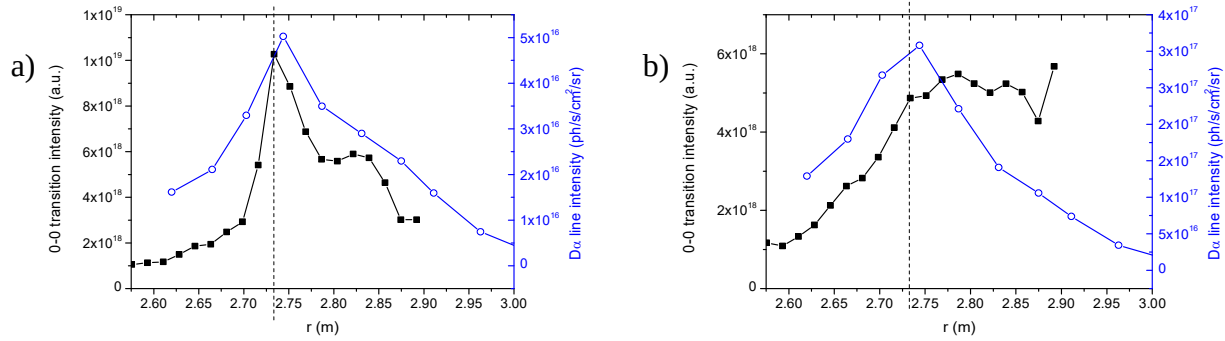
Fig. 4. Spatial distributions of the radiation intensity of the 0-0 molecular transition (black squares) and D$_\alpha$ (blue circles)at the same time: a) t = 10 s, b) t = 15 s (#94767), dashed line denotes strike point position.
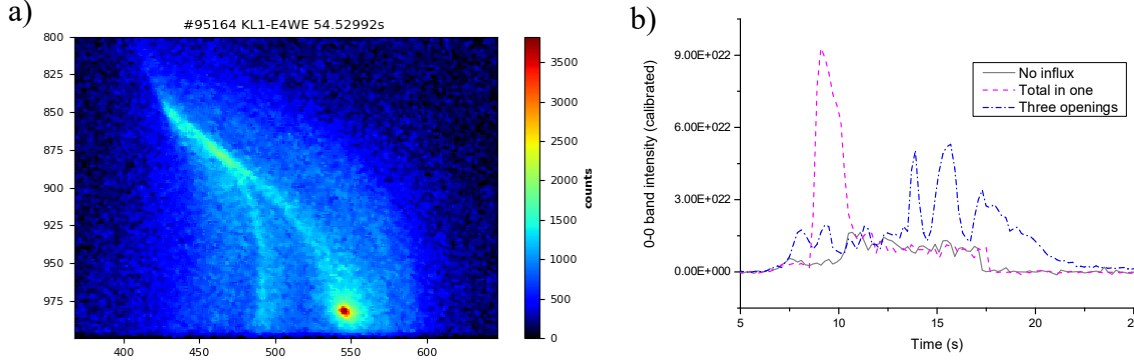

Fig. 5. Results of gas puff into the divertor COS collection angle: a) camera-measured intensity of the D$_\alpha$ line in pulse #95164 b) comparison of the 0-0 transition intensity evolution in three pulses: #95159, #95160, #95163.

The tritium analysis is very complex, because even strongest lines of the 0-0 transition blend with other lines (see figure 1). Preliminary results for the flat density RF heated L-mode pulse (#98594, B = 2.4 T, I = 2.4 MA, auxiliary heating power RF 2 MW) show that the spatial distribution 0-0 band intensity is similar to the one in low-density part of the D$_2$ #94767 pulse, with very high rotational temperature, close to 5000 K. This value may be overestimated, because only six strongest lines with low upper energy difference between the lowest and highest (~1000 cm^{-1}) could be used for the Boltzmann plot. Refining the analysis is complicated by the very limited available molecular data, because only one publication analyzing pure tritium FB spectrum exists in literature [7].

To summarize, the measurements for all isotopes of hydrogen confirm the findings of Sergienko et al [5] in deuterium: in JET-ILW the Fulcher Bands have completely different vibrational and rotational population distributions than in the carbon machines, with high rotational temperature and high intensity of the 0-0 transition. The spatial distribution of the molecular radiation intensity has two different shapes – sharp peak close to the strike point for low-density plasma and much broader peak shifted outwards away from strike point for higher density, with the threshold dependent on used hydrogen isotope and other plasma parameters. We also present an attempt to calibrate the deuterium FB radiation vs the number of particles injected into the plasma.

[1] K. Verhaegh et al, Nucl. Fusion **61** (2021) 106014 [2] M. Groth, Nucl. Mat. Energy **19** (2019) 211-217, [3] A. Perek et al, Nucl. Mat. Energy **26** 100858 (2021) [4] A. Pospieszczyk et al, J. Nucl. Mat **337–339** (2005) 500–504 [5] G. Sergienko et al, J. of Nucl. Mat. **438** (2013) S1100 [6] S. Brezinsek et al, J. Nucl. Mat **363–365** (2007) 1119–1128 [7] Dieke & Tomkins, Phys. Rev. **76** (1949) 293-289.