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Molecular ND Band Spectroscopy in the Divertor Region of Nitrogen Seeded JET Discharges

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Abstract. In this contribution we present OES measurements in the JET tokamak of the deuterated NH (ND) radical and the correlation between results of those experiments and measurement of ammonia production. The observation region covers most of the divertor and its outer throat. Measurements are performed in different magnetic configurations. The results include temporal and spatial dependence of the molecular emission intensity and study of the emission band shape (vibrational and rotational temperatures) during different JET pulses, with or without nitrogen seeding. Results are a step towards the understanding of nitrogen-containing molecule creation and destruction in the divertor plasma.

1. Introduction

Studying the nitrogen plasma impurity is important in fusion plasmas, as this gas is both used for divertor temperature control and has an apparent beneficial effect on confinement. However, it reacts with hydrogen, forming molecules, also stable ones, of which the most prominent is ammonia. In DT plasmas, formation of tritiated ammonia poses several potential issues, e.g. the retention of tritium-containing molecules on metallic surfaces and in the divertor cryo-pumps.

Optical emission spectroscopy (OES) of ammonia is very difficult, because this molecule does not have any strong bands in the visible region. Nevertheless, if by OES we can determine where, when and in which quantity relevant hydride molecules (radicals) are created, the results may give an estimation of the ammonia creation, as those radicals are both precursors for creation of ammonia and results of its destruction. The strongest of hydride bands is a NH radical (or its isotope equivalent) $A^3\Pi$—$X^3\Sigma-$ $\Delta v = 0$ near-UV band at ≈335 nm. Each vibrational transition of this band consists of line-like Q rotational branch and much more distributed P and R branches, with band head at short wavelength. This transition was observed in JET during first experiments with nitrogen seeding in the ITER-Like Wall (ILW) configuration [1].

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[1] See the author list of X. Litaudon et al 2017 *Nucl. Fusion* **57** 102001

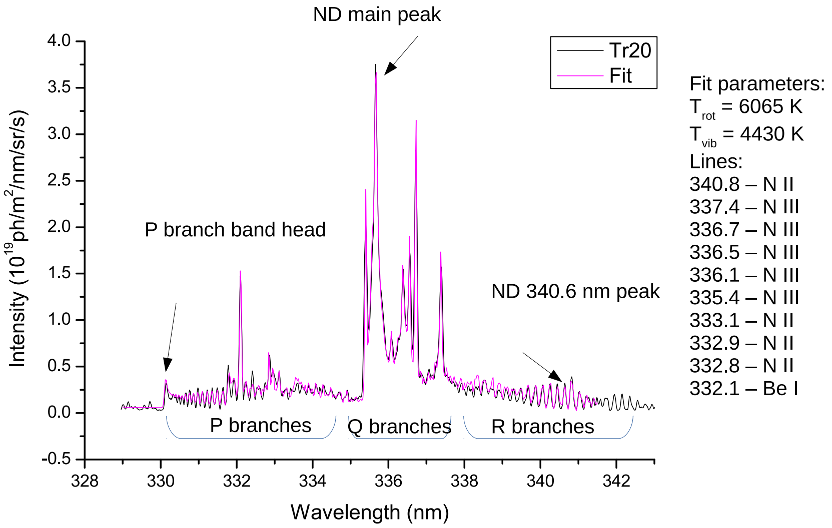

Figure 1. Experimental spectrum (JPL #92143, R = 2.88 m, t = 12.34 s) and fit (most important parameters are shown on the figure).

2. Experiment

Spectra were registered using mirror-link spectrometer KT3 (described e.g. in [2]). This spectrometer has 22 lines of sight covering divertor and part of the outer throat. In the nitrogen seeding experiments the UV detector and 1200 l/mm grating were used, to detect at least partially resolved rotational structure of the ND molecular band.

Experiments were conducted with two different magnetic field configurations: horizontal target, where the outer strike point is on the divertor plate and vertical target, where the strike points are both on divertor throat plates (described in e.g. [3]). In both configurations the ND spectra were visible, although with different intensities. Nitrogen seeding was starting after the formation of the X-point and switching on the NBI heating. Some nitrogen (and ND) was visible before seeding started, and this is called in this contribution a “legacy” phase, where the nitrogen present in the plasma is a “legacy” from previous pulse.

3. Synthetic spectrum

Synthetic molecular spectrum was created with the help of PGOPHER code [4] with diatomic molecular data taken from [5]. Vibrational transitions from 0-0 to 3-3 were taken into account. The exported wavelengths, energy levels and Einstein factors for each transition were used for creating a fitting procedure for the experimental spectrum. Free parameters included: rotational and vibrational temperatures, total molecular band intensity, background level and intensities of atomic/ion lines overlapping the molecular band. An example of the fit is shown in figure 2. Including 10 nitrogen and beryllium lines is sufficient for such strong ND spectrum, but the number of lines has to be increased if recordings with relatively weaker ND bands are to be fitted – there is also a weak N III line overlapping the main 0-0 Q branch.

Fortunately, fitting the whole spectrum may be not necessary for estimating the band intensity or temperatures. Study of the experimental and synthetic spectrum reveal some features which can be used for quick estimation of those values. In the case of ND transition obvious features for total band intensity are amplitudes of Q branches of the vibrational transitions (especially 0-0), but as figure 2 shows, they depend on both rotational and vibrational temperatures. Also, there are many nitrogen lines overlapping the center peaks (figure 1). A better choice is one of composite peaks from R branch, located at 340.6 nm, which amplitude for temperatures above

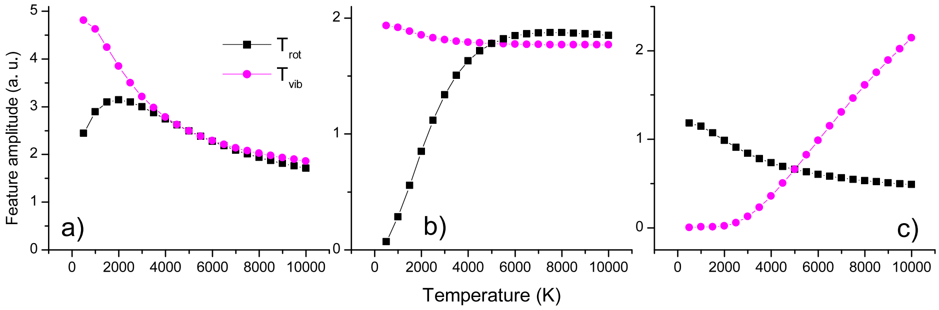

Figure 2. Temperature dependence of a a) main Q branch peak amplitude, b) 340.6 nm feature c) P band head to 340.6 nm feature ratio. For each temperature curve the other temperature is set at 5000 K.

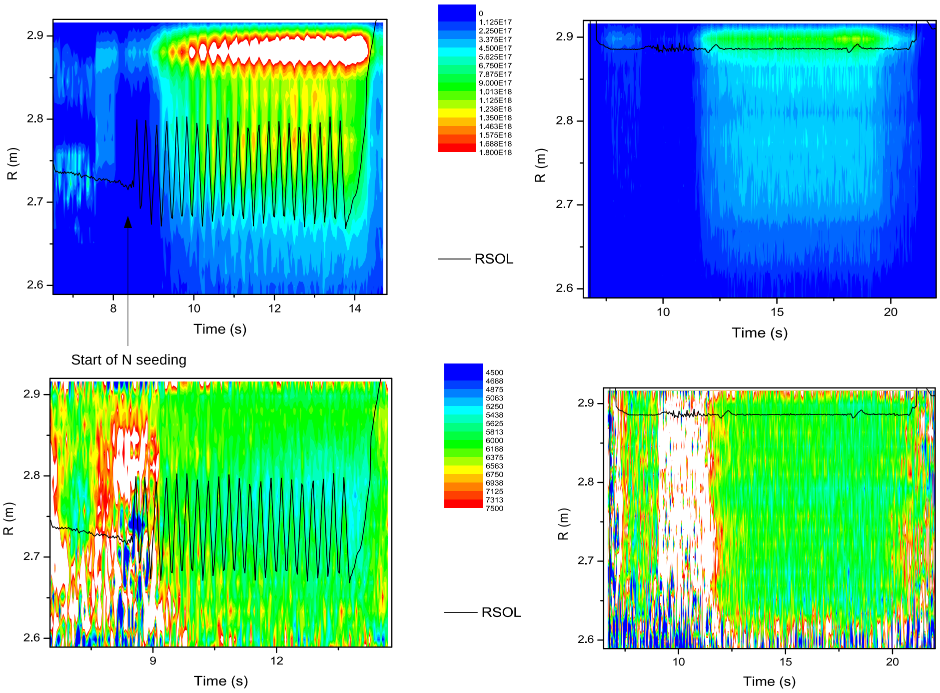

Figure 3. Top: intensity distribution for HT (left) and VT (right) configurations. Bottom: corresponding rotational temperatures for both experiments. Black line (RSOL) denotes position of the outer strike point.

4000 K is nearly independent on any of the temperatures. Short wavelength band head (P branch of 0-0) depends very strongly on rotational temperature, and its ratio to the 340.6 nm peak can be used for T_{rot} estimation.

4. Results

Estimations of total band emission (which is proportional to density of excited molecules) and rotational temperatures were made from amplitudes of the chosen spectral features (340.6 nm and 330.1 nm) with the background estimated from radiation at 329.9 nm. Resulting spatio-temporal distributions for JPL #92143 and #92503 are shown in figure 3. The density of excited ND radicals is much higher in the case of horizontal target experiment, the band intensity is higher by factor of 3. In both cases the intensity is highest at the outer throat of the divertor,

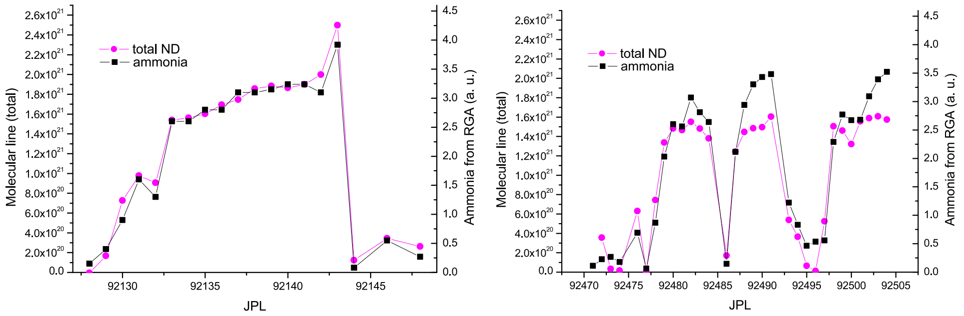

Figure 4. Total ND intensity during JET pulse compared to total ammonia production during the pulse. Left – horizontal target experiment, right – vertical target experiment.

where the N_2 is puffed from. There is a dip in emission between the divertor plates and the throat, and definite dependence on the location of the strike point or, in fact, the separatrix, as the recorded band intensity is a result of the integration along the spectrometer line of sight. The intensity is highest in the seeded part of the pulse, but there is also a time during and just after the X-point formation, when the strike point glides along the vessel walls releasing the adsorbed nitrogen, when ND band emission is visible as well (legacy phase). The rotational temperature distribution is remarkably uniform – for most places and times T_{rot} is between 5600 and 6300 K. There seems to be a lower temperature region just outside the separatrix visible in the horizontal target experiments, but the explanation of this phenomenon is still unclear.

Main value of ND radical plasma content measurement is that it can serve as an indicator for the ammonia production in the plasma. To show that such a correspondence exists the total (spatially and temporally integrated) ND intensity was compared to the total ammonia registered by RGA (Residual Gas Analyzer, [5]), keeping the same scale for vertical and horizontal target experiments. Figure 4 shows, that the results are promising – the ratio is nearly constant and only for a few pulses difference exceeds 10 %. Those discrepancies can be explained taking into account, that the observed region is only a part of area where molecules can be created and in the case of vertical target relatively more molecules can be created in unobserved region.

5. Conclusions

Observation and analysis of nitrogen seeded pulses in JET show that the ND radical radiation may be used as an estimate of ammonia production. Analysis of the synthetic spectra yields also a procedure for a quick estimation of T_{rot} and total intensity of ND band, at least in conditions of JET divertor region.

Acknowledgements

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