

## TEMPERATURE DETERMINATION OF A COLD N<sub>2</sub> DISCHARGE PLASMA BY THE FIT OF THE EXPERIMENTAL SPECTRA WITH THE SIMULATED EMISSION SPECTRA

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*Abstract.* We have had obtained the temperature of a cold hollow cathode electric discharge (HCED) plasma by fitting the experimental rotational spectra of the vibrational-rotational N<sub>2</sub> first negative system (FNS) and of second positive system (SPS) sequences, with the simulate spectra of the same plasma. With the accordance of the rotational temperature from different rotational transitions, with an accuracy of 10%, we found a local thermodynamic equilibrium (LTE) in a cold HCED plasma.

*Key words:* plasma spectroscopy, computational physics.

### 1. INTRODUCTION

Nitrogen plasma is a very important tool in treatment of different material surfaces and also in the study of several atmospheric and physical and chemical medium processes. One of the most important parameter in the plasma tool is the gas temperature ( $T_g$ ). The electronic temperature ( $T_e$ ) is, generally, more greater than gas temperature, while the rotation temperature ( $T_r$ ) has, practically, the same value as the last one [1, 2].

On these reason we have determined the rotation temperature, by the fitting the experimental spectra of the FNS and SPS from a cold HCED in N<sub>2</sub>, with the same spectra simulated.

### 2. EXPERIMENTAL

Experimental spectra where obtained from a molecular nitrogen plasma, produced in a HCED device presented by the authors in a early published paper [3].

The experimental data were achieved on a computer by using a leading spectral system consisting of a SPM-2 Zeiss 650 tr/mm monochromator coupled with a EMI-9558 QB photomultiplier and a data acquisition system. The voltage was placed in the range 200–400 V, the gases pressures in the range of 0–8 Torr and the current intensity 0–200 mA.

### 3. FUNDAMENTALS OF THE MOLECULAR SPECTROSCOPY

The rotational spectra corresponding to the transitions  $N_2^+(B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+)$  FNS and  $N_2(C^3\Pi_u \rightarrow B^3\Pi_g)$  SPS were fitted using synthetic spectra following the steps:

1. Upper and lower energy level corresponded to the implied transitions:

$$W_{nvJ} = W_{el} + hc[G(v) + F(v, J)], \quad (1)$$

where the vibrational term is:

$$G(v) = \omega_e \left(v + \frac{1}{2}\right) - \omega_e x_e \left(v + \frac{1}{2}\right)^2 + \omega_e y_e \left(v + \frac{1}{2}\right)^3 \quad (2)$$

and the rotational term:

$$F(v, J) = B_v J(J+1) - D_v J^2(J+1)^2, \quad (3)$$

$$B_v = B_e - \alpha_e \left(v + \frac{1}{2}\right). \quad (4)$$

In the equations (1)–(4) the symbols have the following significance:  $v$  is the vibrational quantum number,  $J$  is the rotational quantum number,  $x_e$  and  $y_e$  are the anharmonicity constants,  $\alpha_e$  characterize the vibration-rotation interaction,  $B_v$  and  $D_v$  characterize each vibrational level.

The spin-orbit interacting energy:

$$\Delta W = A\Lambda\Sigma, \quad (5)$$

which for FNS levels is zero ( $\Lambda = 0$ ), and for SPS levels has a neglected value [4].

2. The wave number calculation:

$$\tilde{\nu}_R = \tilde{\nu}_0 + G(v') - G(v'') + F(v', J) - F(v'', J-1), \quad (6)$$

$$\tilde{\nu}_Q = \tilde{\nu}_0 + G(v') - G(v'') + F(v', J) - F(v'', J), \quad (7)$$

$$\tilde{\nu}_P = \tilde{\nu}_0 + G(\nu') - G(\nu'') + F(\nu', J) - F(\nu'', J + 1), \quad (8)$$

where  $R$ ,  $Q$ ,  $P$  represents those three branches correspond to the selection rules, respectively  $\Delta J = +1$ ,  $0$  and  $-1$ .

3. The relative intensity of a rotation spectral line is described by the follow relationship:

$$I_{\nu'J',\nu''J''} = \text{const.} \times C_{J'} S_{JJ''} \nu_{\nu'J',\nu''J''}^4 \exp\left[-\frac{hc}{k_B T_{rot}} F(\nu', J')\right], \quad (9)$$

where  $S_{JJ''}$  is the Hönl-London factor which easily can be see in [5, 6], and  $C_{J'}$  is an alternating coefficient in the distribution intensity in a vibration band, which depend on the nuclear spin  $I$ , which in the nitrogen molecular case ( $I = 1$ ) are the values  $(I + 1)/(2I + 1) = 2/3$  for the symmetric levels and respectively  $I/(2I + 1) = 1/3$  for the asymmetric levels.

4. Simulation of the intensity in the rotational structure of the vibrational band:

$$I_{sim}(\lambda) = \sum_{J', J''} I_{\nu'J',\nu''J''} P(\lambda, \lambda_{\nu'J',\nu''J''}), \quad (10)$$

where  $P(\lambda, \lambda_{\nu'J',\nu''J''})$  represents the spectral line profile. In our case the apparatus spectral width is more larger then the plasma broadening spectral line (Doppler, Stark). The profile function is assumed to be of a Gaussian tip:

$$P(\lambda, \lambda_0) = \text{const.} \times \exp\left[-\frac{(\lambda - \lambda_0)^2}{\delta\lambda^2} \ln 2\right], \quad (11)$$

where  $\delta\lambda$  is the full width at half maximum of the line and in our case were approximate  $2 \text{ \AA}$ .

5. The fit of the simulated spectra with the experimental spectra was made by the  $\chi^2$  function minimized:

$$\chi^2 = \sum [I_{exp}(\lambda) - I_{sim}(\lambda)]^2 \quad (12)$$

having the rotation temperature as a fitting parameter.

#### 4. RESULTS AND DISCUSSIONS

On the Fig. 1 we can see a nitrogen spectra from the molecular nitrogen HCED, containing the FNS and SPS bands.

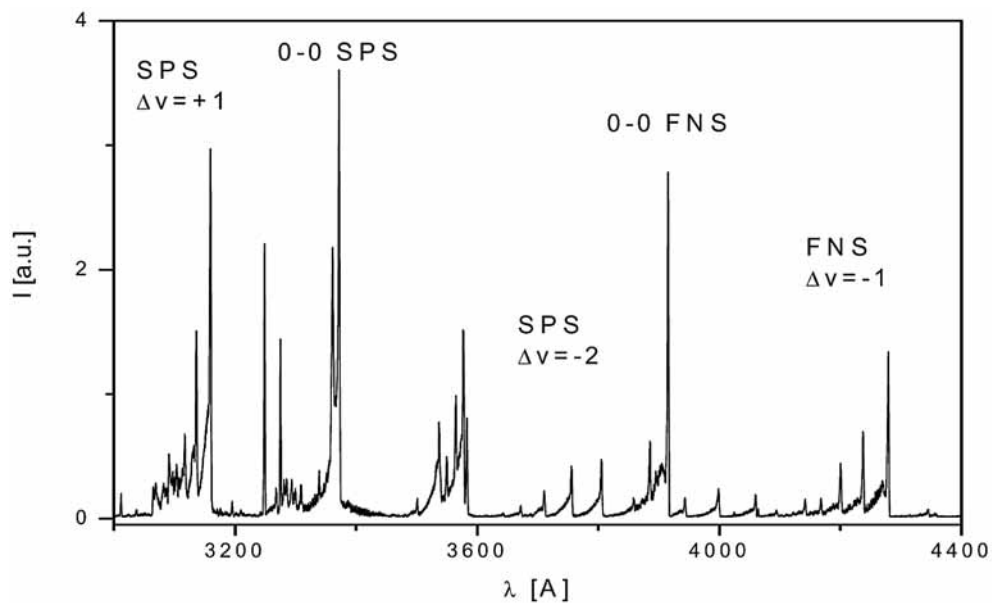
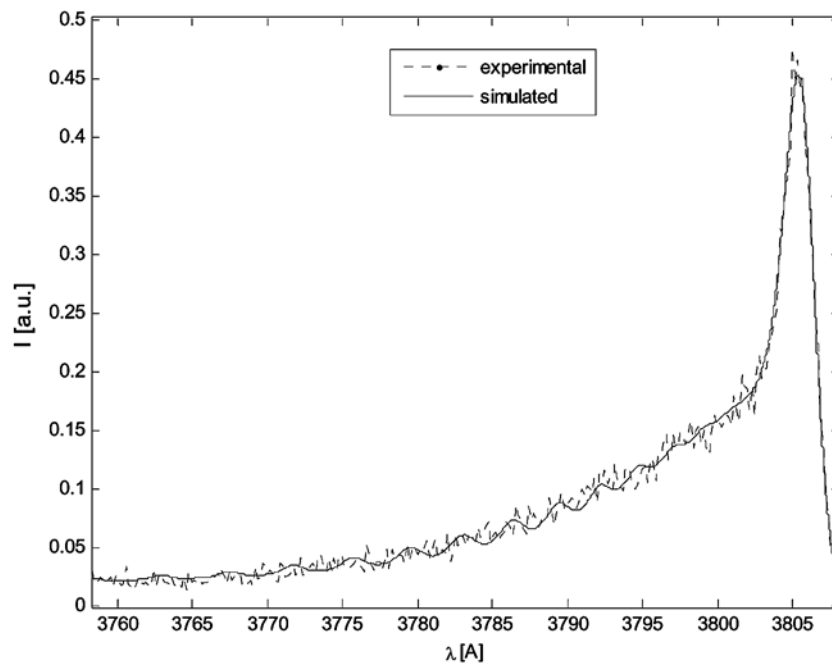


Fig. 1 – Molecular nitrogen spectra in the HCED.

Fig. 2 – Experimental and simulated spectra belonging to 0-2 SPS  $\lambda = 3805$  Å.

Because the rotational structure of the vibrational bands in our conditions can't be resolved, the Boltzmann method for temperature determination is not possible. The rotational temperature was determined by the fit of some vibrational bands belonging to the neutral nitrogen molecule SPS  $v'-v''$ : 0-2, 1-3, 1-0 and to the ionic nitrogen molecule FNS,  $v'-v''$ : 0-0, 0-1. The vibrational bands were chosen in a such a way that their baseline to be not influenced by the neighborhood band.

In Figs. 2 and 3 are represented on the same picture the experimental and the simulated spectra for the 0-2 band  $N_2(C^3\Pi_u-B^3\Pi_g)$  and the 0-0 basic band belonging to the electronic transition  $N_2^+(B^2\Sigma_u^+-X^2\Sigma_g^+)$ . The comparison of the experimental and simulated spectra shows a good fit, on Fig. 3 the alternating intensity of both spectra is well illustrated. The good quality of experimental spectra fit is given also by the relative standard deviations of the rotational temperature which in general, is of the 10%.

On Figs. 4 and 5 are represented the rotational temperature evolutions versus the intensity current of the electric discharge, temperatures determined by the fit of SPS respectively FNS bands. The rotational temperatures determined with the spectral band belonging to the neutral nitrogen molecule have very close values (Fig. 4). This result suggests conclusion that the distribution of the rotational level population satisfies the partial local thermodynamic equilibrium.

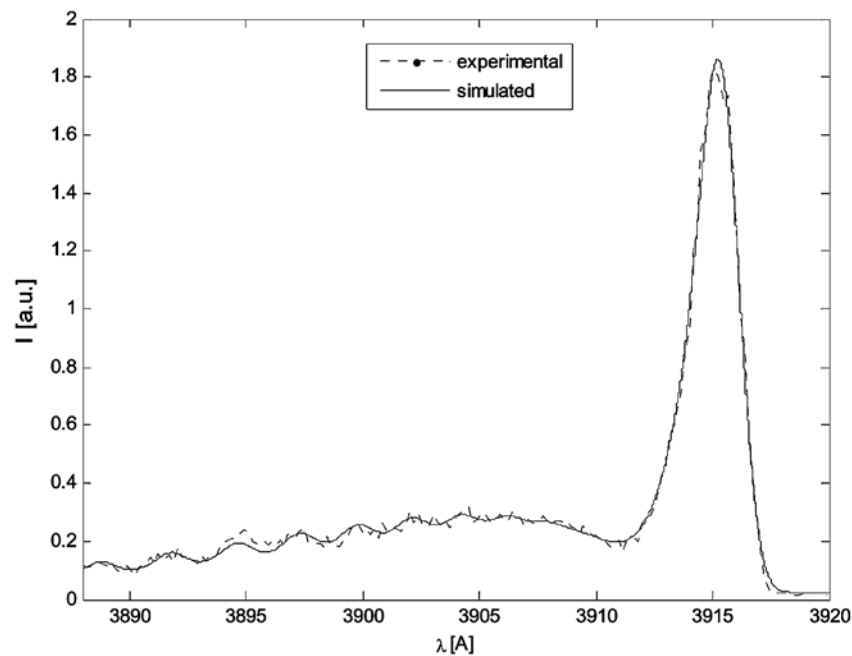


Fig. 3 – Experimental and simulated spectra belonging to basic band 0-0 FNS  $\lambda = 3914 \text{ \AA}$ .

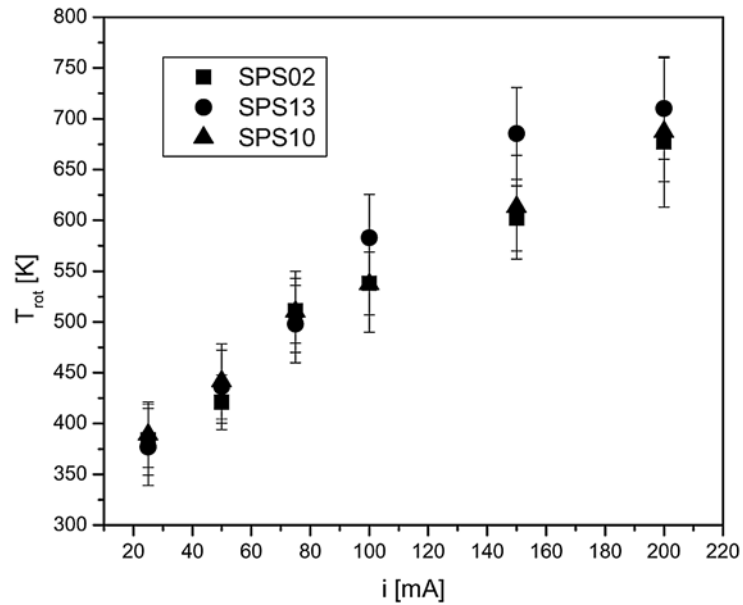


Fig. 4 – Rotational temperature determined from several SPS bands *versus* electric discharge electric current intensity.

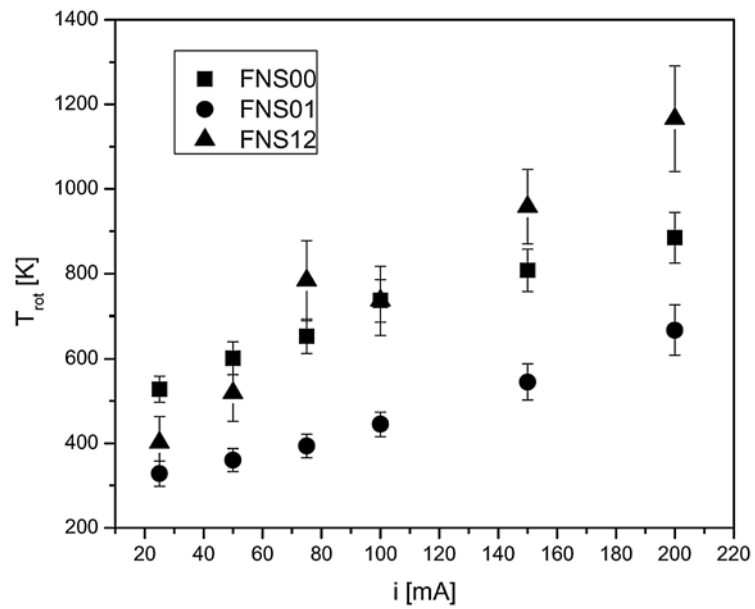


Fig. 5 – Rotational temperature determined from several FNS bands *versus* the discharge electric current intensity.

The rotational temperatures resulting from the several bands analysis of the ionic nitrogen molecule are quit different. As we can see from Fig. 5 rotational

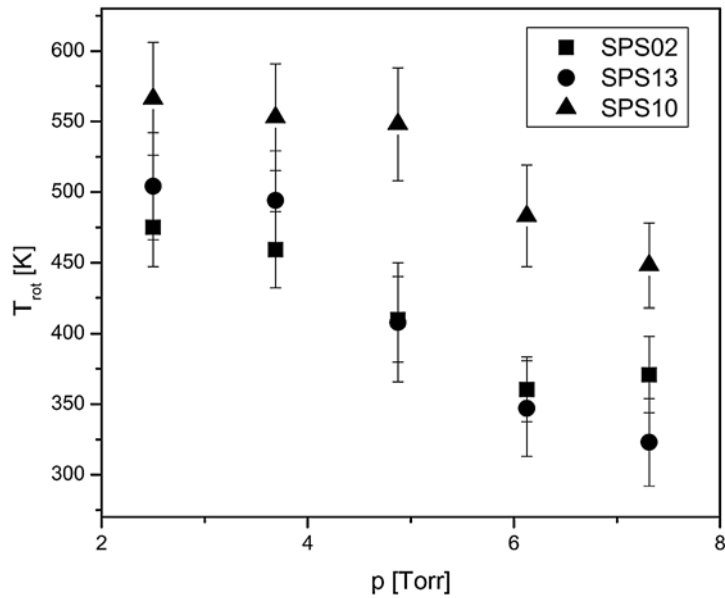


Fig. 6 – Rotational temperatures *versus* the gas pressure (SPS bands).

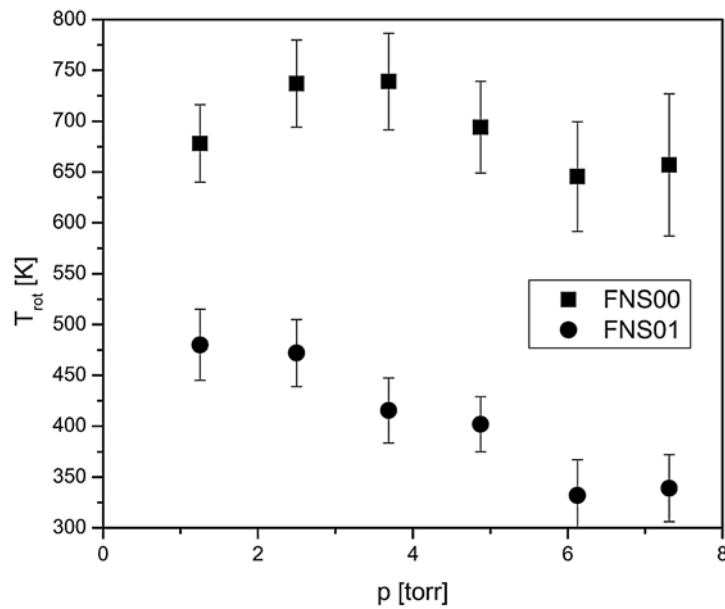


Fig. 7 – The rotational temperature *versus* gas pressure (FNS bands).

temperature determined with the 0-1 FNS spectra are much smaller than the other, which also are not closed. This result suggests the fact that the rotational levels of ionic molecule, in this case are not in the partial LTE.

The dependences of the rotational temperature on the discharge pressure gas are illustrates on Figs. 6 and 7. Analyzing the both evolutions we see that in the case of the neutral nitrogen molecule, the rotational temperatures determined by using the 0-2 and 1-3 SPS spectra, practically coincide (in the limit of the experimental errors). The SPS (1-0) spectrum and his rotational temperature not obey this behavior due to, probable, of some self absorption phenomena on his lower level.

In the case of the nitrogen ionic molecule, between the rotational temperatures determined by using the (0-0), (0-1) FNS spectra is a very much discrepancy (Fig. 7). In this situation we have not the case of a partial LTE.

## 5. CONCLUSIONS

Rotational temperature was determined in a  $N_2$  hollow cathode electric discharge plasma, by emission spectroscopy. The temperatures went determined by numerically simulation of the molecular rotational bands belonging to SPS and FNS sequences, and comparing these with their experimental spectra.

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