

Estimation of the plasma temperature by using the resolved spectrum of N_2^+

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Abstract. This publication analyzes the problems of estimating the gas temperatures in the nitrogen-containing plasma in the temperature regions between 4 and 9 kK. Problems of low and high resolution molecule bands spectroscopy and temperature derivation is discussed and the proposition of the quick procedure is presented. Its validity is tested by comparison of the temperatures derived from different molecular bands by the help of the Boltzmann rotational structure diagrams. The perturbation in the molecular spectrum is exploited to choose the most easily resolved spectral lines.

1 Introduction

Estimating the plasma temperature is one of the basics of plasma diagnostics, together with the population densities and velocity of the gas flow. In most cases of low-temperature plasmas the temperature measurements are based on the thermal equilibrium in some subsets of plasma (e.g. Maxwell velocity distribution, Boltzmann energy distribution in some levels, etc.)

Most popular plasma temperature measurements in plasma arcs are based on Boltzmann plots of atomic or ionic levels or Saha balance for two consecutive stages of ionization, but the validity of such measurement is limited by the visibility of atomic lines originating from higher-excited levels. In the case of the argon or helium based arc plasmas this means the measurements are valid only for temperatures higher than 7–8 kK.

For plasma temperature lower than 8 kK measurements of the temperature start to get quickly more difficult, especially because of the problems with local thermal equilibrium. Even if the atomic lines are still visible, the population densities of atomic levels are no longer determined by collisions with electrons, due to the big energy separations between levels, too big for energy of the electrons. There are still equilibrium subsets to be found, but for vibrational and rotational levels of molecules. Popular approximation is that the distribution of the populations of rotational levels reflect the gas temperature (as given by Dalton law or Maxwell distribution of heavy particle velocities), and the vibrational temperature is termed excitation temperature and connected, at least partially, with energy distribution of electrons.

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2 Possible approaches to plasma temperature measurements using molecular bands

Determining the plasma temperature using the molecular spectroscopy can be done either by low-resolution or by high-resolution approach. For both approaches the energies and line strengths of the molecular lines have to be known.

In the high resolution situation creating the simple Boltzmann diagram is possible. In the low resolution approach modeling of the full molecular spectrum have to be done, and then the temperature parameter adjusted to obtain the best fit of the theoretical spectrum to the experimental one [1]. The problem is, that in the case of molecular band overlaps all the spectra present have to be taken into account, and also, the theoretical data should be exact for all molecular sublevels, to obtain the proper shape of the spectrum (in the high-resolution case some of the lines can be omitted).

The problems with lower-resolution approach in the temperature regions discussed in this publication is also, that the overall shape of the molecular bands does not change significantly between for example 6 kK and 7 kK. In this case the shape depends much more on, between others, slight miscalculation of the rotational sublevels energies, than on the rotational temperature. Taking into account the bigger wavelength region would be possible also, but there is an overlap with a strong CN band and some nitrogen lines.

2.1 Structure of the nitrogen first negative bands

The structure of the N_2^+ 3900 and 4200 Å first negative bands is determined by quantum numbers of the electronic B and X levels. The levels are described as the Hund b case, with weak coupling between S and molecular axis, Λ and rotation coupled give K, so energies thus are:

$$F_1(K) = BK(K+1) + \frac{1}{2}\gamma K, \quad \text{for } J = K + \frac{1}{2} \quad (1)$$

$$F_2(K) = BK(K+1) - \frac{1}{2}\gamma(K+1), \quad \text{for } J = K - \frac{1}{2} \quad (2)$$

The intensity of the lines are determined by Hönl-London factors. The studied bands are the ${}^2\Sigma - {}^2\Sigma$ transitions, so the factors in their case are[2]:

$$S_J^R = \frac{(J''+1) - \frac{1}{4}}{J''+1} \quad S_J^Q = \frac{2J''+1}{4J''(J''+1)} \quad S_J^P = \frac{J''^2 - \frac{1}{4}}{J''} \quad (3)$$

Unfortunately, these equations do not describe the N_2^+ spectrum completely, as there is the significant perturbation of the B vibrational sublevel ($v=0$) by high ($v \approx 11$) vibrational sublevels of electronic level A[3], so the energy calculation is even more difficult (see Fig. 2).

The slight dependence of the low resolved band shapes on the rotational temperature can be explained by small wavelength difference between the lines from *P* and *R* branches, originating from very differently excited levels (the difference is of the order of $20J$). The lines themselves can exhibit a relatively strong dependence on temperature, but by their overlap the difference is masked.

3 Experimental setup

The experiment was performed in a Maecker-like wall-stabilized arc, widely used for measuring the atomic and ionic constants [4–6]. The setup was similar to those described in [7], but the

measurements were performed side-on, and the width of one track corresponded to 0.18 mm. Gas mixture was based on helium, with the additions of argon and nitrogen.

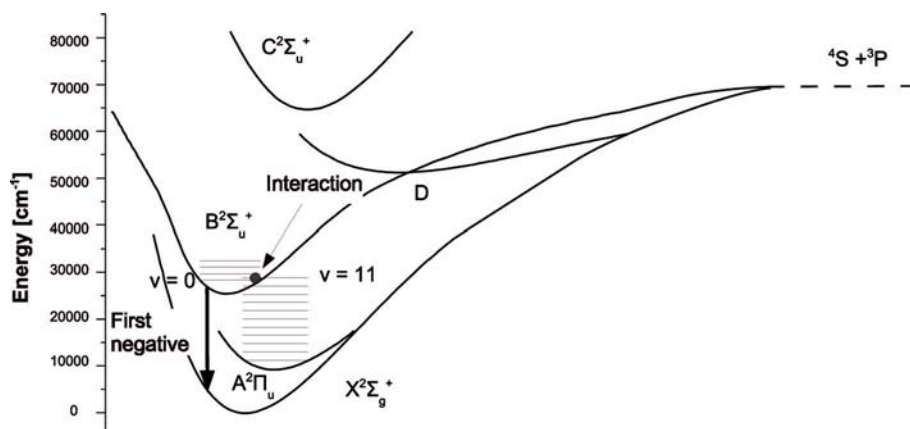


Fig. 1. Energy curves and transitions for N_2^+ molecule - highlighted is the region of the perturbation of B level with higher sublevels of A.

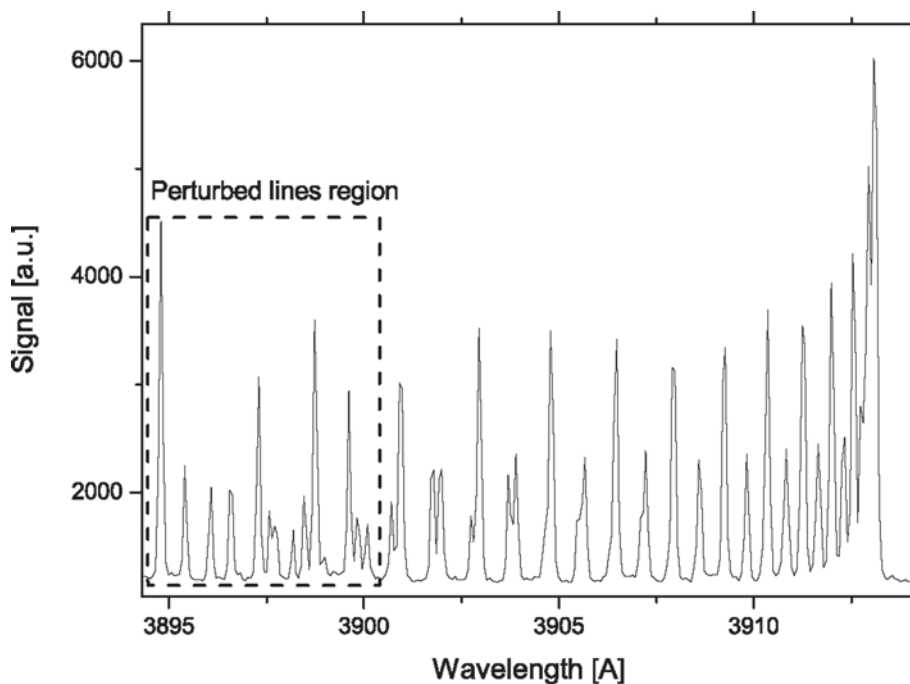


Fig. 2. Example of the experimental data - visible the region of lines perturbed by influence of the nitrogen A electronic level.

The example of the recorded signals is presented in Fig. 2. For the Boltzmann plot were chosen those lines, which could be resolved (with the help of fitting the experimental profiles to the lines).

4 Results

As can be seen in Fig. 3, the resolved molecular lines could be reasonably fitted, giving the values of rotational temperatures for different plasma regions. To be more sure that the resolving of the molecular lines does not add the significant amount of error to the resulting of the temperature values, the same procedure was applied to two molecular bands of N_2^+ , both originating from the same higher vibrational sublevel, but with different wavelength spacings between the molecular lines (0 – 1 band at 4200 Å is easier to resolve than 0 – 0 band at 3900 Å). For comparison, the temperature was calculated, as well, taking into account only two lines, one of which due to the perturbations is shifted so much, that the lines are completely separated. As is presented in Fig. 4, the temperature values show reasonable agreement, which supports the idea of using those two lines for quick estimation of plasma temperature.

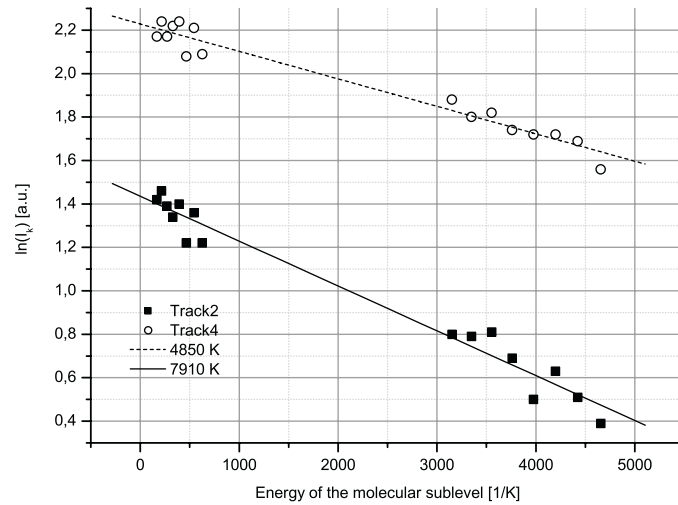


Fig. 3. Boltzmann plots for two different plasma regions.

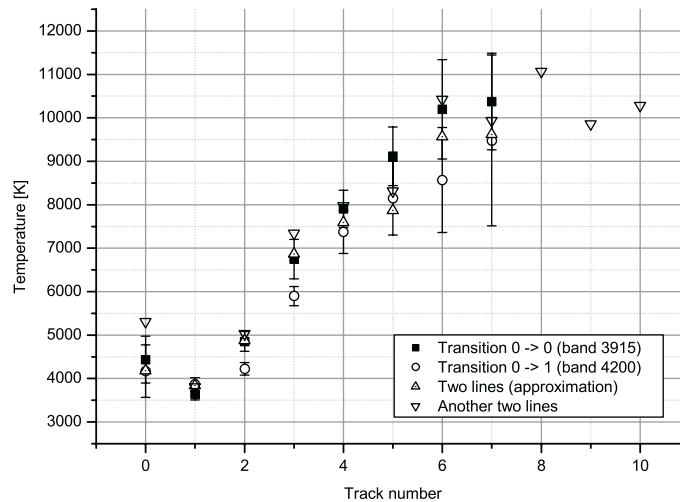


Fig. 4. Temperatures calculated from Boltzmann plots of different nitrogen bands and from two chosen line ratios.

5 Conclusions

Modeling of the unresolved N_2^+ spectrum is not very reliable for obtaining the rotational temperatures for regions with temperatures higher than 3 kK, because the overall shape of the band changes then only very slightly with temperature and the errors are high. This behavior results from overlaps of the lines from P and R branches, where the difference between energies of the upper levels of P and R transitions are of the order of 20 B. Reliable estimation of the rotational temperatures can be performed when the wavelength region taken into account is of the order of 100 Å and more, but this includes modeling many vibrational transitions and in many cases also the neighboring N_2 and CN branches.

Resolving the P and R branches gives much more reliable estimation of the rotational temperature. Unfortunately, they are not easily totally resolved, so the analysis is done by fitting overlapping experimental profiles to the experimental spectrum, which is time-consuming and introduces some errors. Quick estimation can be done using the P -branch lines shifted by interaction of this level with A N_2^+ level, because they are much better separated from their R neighbours.

References

1. H. Nassar, S. Pellerin, K. Musiol, O. Martinie, N. Pellerin, J.-M. Cormier, J. Phys. D: Appl. Phys. **37**, 1904 (2004)
2. R.S. Mulliken, Rev. Mod. Phys. **3**, 89 (1931)
3. F. Michaud, F. Roux, S.P. Davis, A.-D. Nguyen, C.O. Laux, J. Molec. Spectr. **203**, 1 (2000)
4. J. Musielok, W.L. Wiese, G. Veres, Phys. Rev. A **51**, 3588 (1995)
5. V. Helbig, K.-P. Nick, J. Phys. B **14**, 3573 (1981)
6. A.T.M. Wilbers, G.M.W. Kroesen, C.J. Timmermans, J. Q. S. R. T. **45**, 1 (1991)
7. I. Ksiazek, E. Pawelec, Contrib. Plasma Phys. **43**, 73 (2003)