

Simulation of the OH emission molecular spectrum to determine the plasma temperature and the influence noise to signal ratio on the temperature values

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The OH system ($A^2\Sigma^+ - X^2\Pi_i$) molecular emission spectrum is frequently observed in plasma sources containing water. We have simulated the spectrum of (0,0) band of this system from 3064 Å for different rotational. The influence of the noise to signal ratio has been studied, if the noise to signal ratio is about 10% we found an error of 6% at temperature 3000K and 10% at 6000K.

1. Introduction

The violet system of OH molecule is a good tool for diagnosing plasmas containing this molecule, the molecular constants and the lines structure are well-known, and it is present in most of the plasma sources containing hydrogen and oxygen for a temperature between 1000K and 6000K.

Pellerin (1996) and De Izarra (2000), has simulated UV OH system to measure temperature in plasma [1] and [2]. Salloum (2002), uses this system for temperature measurements in RF plasmas Quasi-thermic [3].

In the previous publications, we have proposed a numerical method based on the simulation of molecular spectrum for studying the distribution temperature in modified arc Maeker[4] and[5], and in transferred arc[6]. To determine N_2^+ / N_2 ratio and the temperature distribution in Glidarc [7], we have made the simulation of both systems first negative and second positive one simultaneously.

In this paper, we have used this method based on the simulation of the (0,0) band of UV OH molecular system. The method proposed permit to evaluate, by comparing point to point a real

spectrum with the simulated one, temperature and apparatus function, approximated by the gauss function (the half-width at 1/e height). Moreover, it is shown, by noised spectra simulation, the influence of noise to signal ratio at the calculated temperature values.

2. The OH molecular violet system

The violet system of molecule diatomic OH corresponds to radiative transitions between the $A^2\Sigma^+$ and $X^2\Pi_i$ electronic state at 4,046 eV and 0 eV respectively (figure 1). We are interested in the (3064.8Å, 3100Å) spectral range covering the (0, 0) band. The coupling is type (b) Hund case for the $2\Sigma^+$ state and near of (a) Hund case for $2\Pi_i$ state. The absolute rotational emission line intensity of the molecule is given by

$$\varepsilon_{ul} = C \sigma^4 \cdot S_{J'J''} \cdot \exp\left[-\frac{hc F(J')}{KT}\right] \quad (1)$$

Where C is a normalization constant, σ is the wave number, $S_{jj''}$ is the Hönl-London factors, h and c are the conventional physical constants, $F(J')$ is the spectral terms and T is the temperature (mark (') concerns the lower spectral term and the mark (") is for the upper one).

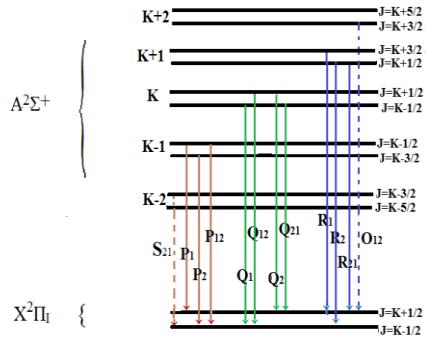


Figure 1: Transition between both electronic States $A^2\Sigma^+$ and $X^2\Pi_i$

Line S_{21} and O_{12} are forbidden transitions (very weak intensities)

3. Numerical simulation

Line intensities are calculated when a state of thermodynamic equilibrium is fully reached and the corresponding temperature of the gas, considered from a macroscopic and thermodynamic point of view, are the same. In reality, within laboratory plasmas, we usually have to deal with a local thermal equilibrium state instead of thermodynamic equilibrium state.

It is possible, when the population of discrete energy levels follow Boltzmann's Law, to attribute a corresponding temperature for each corresponding energy distribution; electronic, T_e , vibrational T_v and rotational T_r . In a non-equilibrium plasma T_r , T_v and T_e may differ from the kinetic temperature T_g of heavy species. Taking into account the strong coupling between translational and rotational energy states, the temperature derived from experiments is, in a general case, close to the gas kinetic temperature [10] and [11]. Thus, T_g can be deduced from T_r , measured by using the rotational structure of molecular spectra.

All the spectral constants are taken from Herzberg [6]. Computed spectrum of individual lines for a given temperature is then convoluted with our

apparatus function approximated by the gauss function whose DX (the half-width at 1/e height):

$$I_0 = \int_{v_0-\varepsilon}^{v_0+\varepsilon} I_\nu \cdot \exp\left[-\frac{(\nu - \nu_0)^2}{DX^2}\right] d\nu \quad (2)$$

Where $\tau = 2.5 DX$ and v_0 is the wave number of the line.

An integrated cell (pixel) of simulated spectrum is chosen according to the cell of experimental spectrum under consideration. We can, following the situation, group several cells in one.

Practically, for each given set of values (DX , Tr), the line intensities of this band are normalized to its maximum. Examples of simulated spectra, normalized to 100. A quick analysis of these simulated spectra shows that the rotational temperature has a great influence on the height of the line as show in figures 2, 3, and 4.

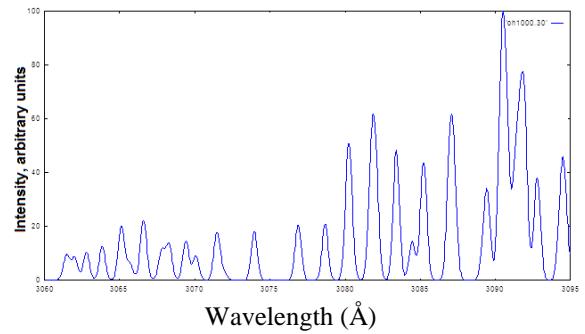


Figure 2: Simulated spectrum with $Tr = 1000K$ and $DX = 3 \text{ cm}^{-1}$.

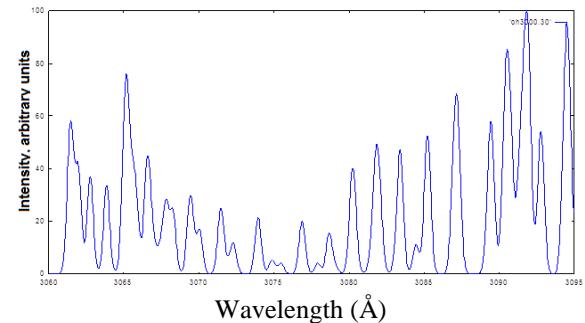


Figure 3: Simulated spectrum with $Tr = 3000K$ and $DX = 3 \text{ cm}^{-1}$

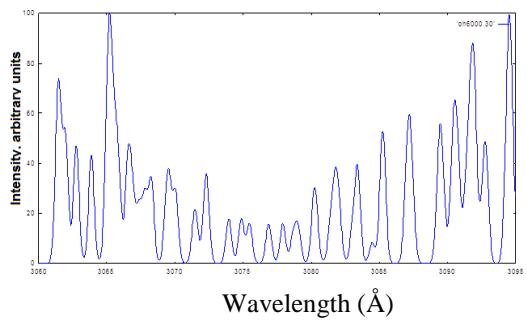


Figure 4: Simulated spectrum with $Tr = 6000\text{K}$ and $DX = 3 \text{ cm}^{-1}$

The apparatus function has essentially influenced the resolution of the rotational line structure as show in figures 5, 6, and 7.

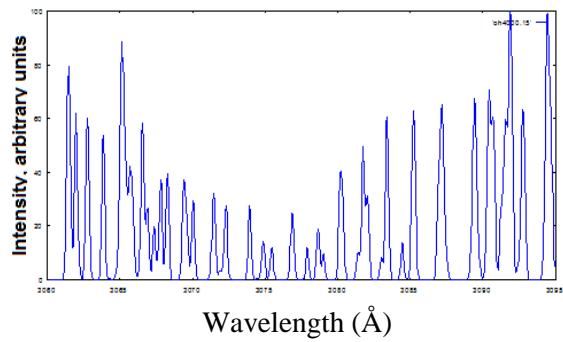


Figure 5: Simulated spectrum with $Tr = 4000\text{K}$ and $DX = 1,5 \text{ cm}^{-1}$

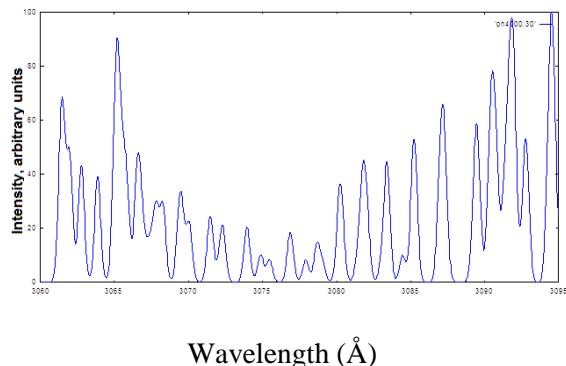


Figure 6: Simulated spectrum with $Tr = 4000\text{K}$ and $DX = 3 \text{ cm}^{-1}$

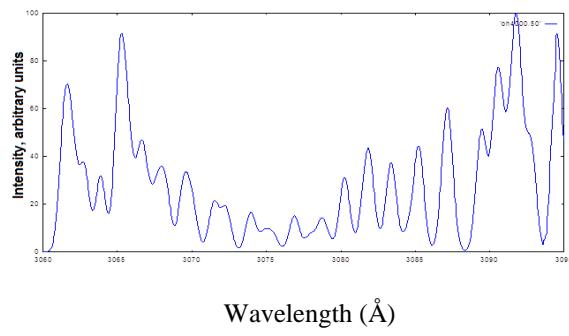


Figure 6: Simulated spectrum with $Tr = 4000\text{K}$ and $DX = 5 \text{ cm}^{-1}$

4. Numerical method for rotational temperature evaluation

To evaluate the temperature from a given real spectrum, we compare this spectrum point-by-point with spectra simulated at different values of DX Tr .

- (i) The measured spectrum was corrected for the continuous background, which was assumed to be linear in the studied spectral range.
- (ii) The experimental spectral intensity was normalized to the maximum value, which was set to 100.
- (iii) The experimental data were compared with that of the simulated spectrum. The minimization procedure was used to minimize $E(T_r, DX)$ as a function of Tr , and DX defined as:

$$E(T_r, DX) = \frac{1}{N} \left[\sum_{i=1}^N (I_i^r - I_i^s)^2 \right]^{1/2} \quad (3)$$

I_i^r and I_i^s are respectively the intensities of the real and simulated i -th pixel of the spectrum containing N points

To test the sensitivity of the temperature estimator, we applied this method when a noisy spectrum was used instead of the experimental one. The synthetic spectra were calculated for known apparatus functions, temperatures, and noise was introduced using a random number generator. Examples of simulated spectra noised are shown in figures 8 and 9 for N/S ratio 20% and 10% respectively.

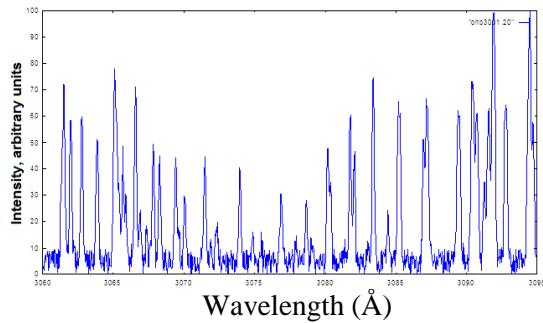


Figure 7: Simulated spectrum with $Tr = 3000K$
 $DX = 1 \text{ cm}^{-1}$ and $N/S = 20\%$

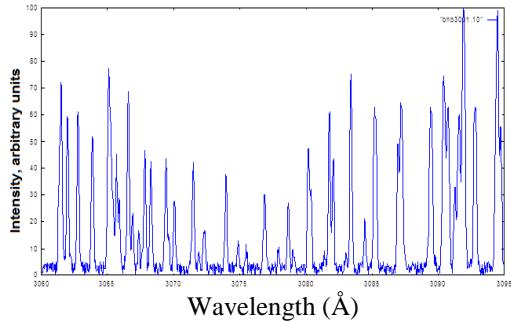


Figure 8: Simulated spectrum with $Tr = 3000K$
 $DX = 1 \text{ cm}^{-1}$ and $N/S = 10\%$.

5. Results and Discussion

Calculations were performed for noise-to-signal ratios N/S equal to 1%, 5%, 10% and 20% and for temperatures of 3000 and 6000 K. The results obtained are given in table 1.

The results are satisfactory, since the relative error in the temperatures is of the same order of magnitude as the noise-to-signal ratio, even if the

last one was relatively high. Figure 9: Simulated spectrum with $Tr = 3000K$ $DX = 5 \text{ cm}^{-1}$ and $N/S = 20\%$.

Table 1. Evolution of the relative error on the temperature with noise/signal ratios

Noise/signal %	$\Delta T/T\%$	
	3000k	6000k
1%	1.5%	3%
5%	4%	7%
10%	6%	10%
20%	11.5%	18.5%

We present in figures 10 and 11 a real spectrum of OH molecule (captured with StellarNet, Inc high resolution ultraviolet spectrometer) and the best simulated spectrum.

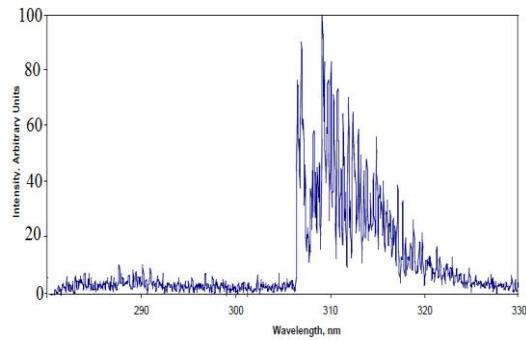


Figure 10: Real spectrum of Polymethyl methacrylate rocket plume taken 0 mm from the nozzle end of fuel grain.

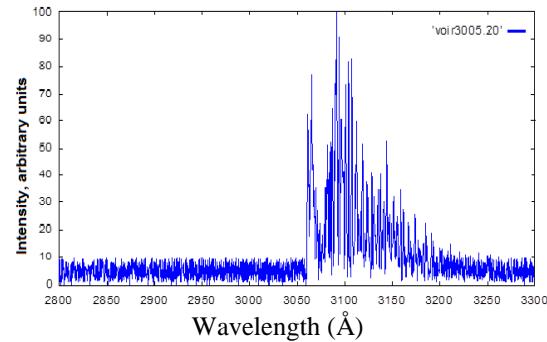


Figure 11: Simulated spectrum with $Tr = 3000K$
 $DX = 5 \text{ cm}^{-1}$ and $N/S = 20\%$.

Given that when the concentration of emitting molecule is relatively weak, the spectrum of molecular emission seems immersed in the continuous background noise. In other words, the ratio noise/signal depends strongly on the molecular concentration, we can therefore, using this method to determine at what temperature the emission is maximum and hence its concentration.

6. References

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