

Improved method for determination of roto-vibrational temperatures from low resolution molecular spectra

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IMPROVED METHOD FOR DETERMINATION OF ROTO - VIBRATIONAL TEMPERATURES FROM LOW RESOLUTION MOLECULAR SPECTRA

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Introduction

One approach developed in the last decades for the determination of molecular roto-vibrational temperatures is to compare experimental spectra with computer simulated spectra. In this way it is possible to obtain the roto-vibrational temperatures even from spectra recorded with low resolution spectral instruments. The reported procedures using computer simulation for determination of rotational and vibrational temperatures uses as information the apparatus profile width (as entry data in the process of simulation) and the recorded spectra should be corrected with the relative spectral sensitivity of the recording chain [1,2]. The subtraction of background and continuous emission should be performed. At least some bands which are strongly dependent on one of the temperatures (thermometric lines) are compared with the experimental spectrum for different values of T_r and T_v parameters until a convenient matching of the spectra is obtained. In case of using the method of thermometric lines the experimental information contained in other bands excepting those taken as thermometric is not used.

The aim of the present work is to study the efficiency of a new computer procedure for comparison between the recorded and simulated spectra, allowing to obtain the temperatures even in the case when the experimental information is not complete. This procedure applies for instance when the apparatus profile width, the relative spectral sensitivity of the spectral system or the background and continuous plasma emission of the spectra are lacking.

Comparison procedure

In this work advantage was taken on the use of many experimental points that exist in the whole spectrum, making possible a fit procedure based on multiple fitting parameters. The lacking information about spectra has been considered as follows:

- a) The width of the apparatus profile is treated as a fit parameter together with the rotation and vibration temperatures.
- b) The dependence on the wavelength of background (B), and of relative spectral sensitivity (S) was assumed (1) to be:

$$B(\lambda) = B_0 + B_1 \cdot \lambda \quad \text{and} \quad S(\lambda) = 1 + S_1 \cdot \lambda$$

This assumption is based on the fact that the spectral range is not too large and a linear approximation is sufficient. The quantities B_0 , B_1 , S_1 are considered fit parameters as well.

The fit parameters are determined by an iterative fitting method applied to normalised simulated and experimental spectra. Because even small shifts in wavelengths are producing significant errors in temperatures the spectra have been preliminary aligned by maximising their correlation coefficient. The main step of the method is the numerical computation of the non-linear system of equations resulted from the condition of minimum for mean standard deviation. In order to accomplish this aim we used an improved variant of standard Newton iterative method.

Results

Spectra have been recorded in the expansion of a cascade arc plasma generated in Ar/H₂/SiH₄ and Ar/C₂H₂ gases. The emission spectra of SiH(A²Δ-X²Π, transitions 0-0,1-1,2-2, spectral range 4050-4250 Å) and CH(A²Δ-X²Π, transitions 0-0,1-1,2-2, spectral range 4200-4420 Å) radicals have been used for temperature calculations. The spectra have been simulated by

using the molecular constants, and transition probabilities given in [3,4]. Typical values of computed temperatures have been, depending on the discharge conditions, T_v=3500-4000 K, T_r=2900-3200 K for silane injected plasma and T_v=2800-2900K, T_r=2800-2900 K for acetylene injected plasma. Typical values for FWHM were in the range of 2-5 Å. Two examples of experimental spectra and their best fit are shown in Fig1.

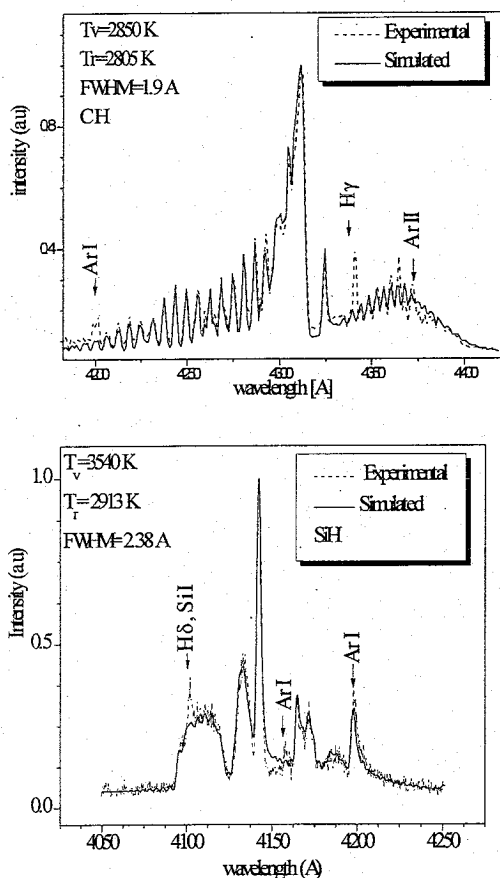


FIG. 1

the same slit width. The errors were found to increase only with 40% when the FWHM is increased from 0.3 to 8 Å, proving the ability of the method to obtain good results even in conditions of low spectral resolution.

Conclusion

An improved procedure for obtaining rotational and vibrational temperatures by comparing the experimental molecular spectra with the simulated spectra is described. It uses a precise many parameters fitting method and it is possible to be applied even in cases when the width of the apparatus profile, the spectral sensitivity of the recorded system are not known. Also a reduced time is required for data processing.

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