Journal of Research in Physics Vol. 28, No. 3, 271-273 (1999)

THE DECONVOLUTION OF SPECTRAL LINE PROFILES OBTAINED BY FABRY-PEROT INTERFEROMETER

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1. INTRODUCTION

The Fabry-Perot interferometer is an instrument with high luminosity-resolution product and is widely used in optical spectroscopy. In addition, it is one of a few spectroscopic instruments for which analytic approximation to its apparatus function is known with a high accuracy. If the spectral source line shape is known, the shape observed by means of Fabry-Perot interferometer can be described as a convolution of spectral source line profile and its instrumental function. At the low perturbing gas pressure, the spectral source line shape is often approximated by well-known Voigt profile $I_V(\lambda)$ which is convolution of the Gaussian $I_D(\lambda)$ and Lorentzian $I_L(\lambda)$ distributions:

$$I_V(\lambda) = I_L(\lambda) \otimes I_D(\lambda) = \int_{-\infty}^{+\infty} d\lambda' I_L(\lambda - \lambda') I_D(\lambda')$$

If we assume that there is no correlation between collisional and Doppler broadening, then the line shape obtained by means of Fabry-Perot interferometer is a convolution of the Airy instrumental function and the Voigt profile. Following Balik (1966), this convolution can be given in an analytical form:

$$I(\lambda) = A\left\{\frac{1}{2} + \sum_{n=1}^{\infty} R^n \exp(-nL)\exp(-n^2 D^2/4)\cos\left[\frac{2\pi n}{\Delta\lambda_s}(\lambda - \lambda_o + \Delta)\right]\right\} \qquad (1)$$

where

$$D = \frac{\pi}{\Delta\lambda_s}\frac{\Delta\lambda_D}{\sqrt{\ln 2}} \; ; \; L = \frac{\pi}{\Delta\lambda_s}\Delta\lambda_L \qquad (2)$$

where: $\Delta\lambda_D$ and $\Delta\lambda_L$ are full halfwidths of Gaussian and Lorentzian fractions, respectively; $\Delta\lambda_s$ is free spectral range of Fabry-Perot interferometer; R is reflectivity of Fabry-Perot interferometer plates; Δ is the shift of the maximum with respect to the unperturbed wavelength λ_o; A is normalizing factor and I is normalized intensity.

The Gaussian fraction of Voigt profile gives the information about gas kinetic temperature of the discharge, while Lorentzian fraction describes the pressure broadening of the spectral line. In order to obtain parameters of the broadening (widths and shifts) it is necessary to apply deconvolution procedure to experimental line profiles.

Until recently, the graphical method for deconvolution of spectral line profiles scanned by piezoelectricaly driven Fabry-Perot interferometer from the relative widths (Platiša et al., 1983) is employed in our laboratory (Kuraica and Konjević, 1992; Šišović et al., 1995). However, we have found that its application is particularly difficult in case of overlapping lines.

In this paper we present a method for deconvolution of overlapping lines caused by two close spectral lines and/or by isotope components spectral lines of an inert gas. This deconvolution method uses software package MS Visual Studio 6.0. To optimize fitting

parameters values, Marquardt-Levenberg algorithm for χ^2 merit function minimisation is applied (Marquardt, 1963).

The method is tested on examples of atomic lines of natural neon. The model profiles match experimental data very well.

2. CALCULATIONS

Let assume that the measurements of line shapes are performed using natural neon which is mixture of ^{20}Ne (90.92%), ^{21}Ne (0.257%) and ^{22}Ne (8.823%) isotopes. In the good approximation the contribution of the ^{21}Ne isotope to the observed intensity can be omitted so that the overall shape is the superposition of two isotope components. The model function, which is fitted to the overall experimental shape, can be written as:

$$I(\lambda) = BL + A\sum_{k=1}^{2} a_k \left\{ \frac{1}{2} + \sum_{n=1}^{\infty} R^n \exp(-nL)\exp(-n^2 D^2/4)\cos\left[\frac{2n\pi}{\Delta\lambda_s}(\lambda - \lambda_0 + \Delta + d_k)\right]\right\} \quad (3)$$

where: BL is the base line value, a_k is the relative intensity of the k-th component of a line ($\Sigma a_k=1$), A is a normalizing factor independent of the wavelength λ, and R is reflectivity of Fabry-Perot interferometer plates. In Eq. (3): $L=(\pi\Delta\lambda_L)/(\Delta\lambda_s)$; $D=(\pi\Delta\lambda_D)/(\Delta\lambda_s(ln2)^{1/2})$; $\Delta\lambda_s$- the free spectral range of the Fabry-Perot interferometer; λ_o- the unperturbed wavelength of the line; Δ- the shift of the maximum with respect to the unperturbed wavelength λ_o; d_k- the isotope shift of the k-th component; $\Delta\lambda_D$ and $\Delta\lambda_L$ are full halfwidths of Gaussian and Lorentzian fractions of the measured profile, respectively. The number n determines accuracy of calculation as well as computing time, but its value can be set on 10, because the array given in Eq. (3) converges rapidly for values of R, D and L expected in laboratory conditions.

The parameters adjusted in fitting to the experimental profiles are: base line BL, normalizing factor A, reduced Doppler halfwidth D, reduced Lorentz halfwidth L and sum of shifts $\Delta+d_k$. The values of these parameters have to be initially estimated. The values for isotope shift d_k could be taken from the literature (Schöber, 1939) when available. The $\Delta\lambda_s$ value is determined by theory of ideal Fabry-Perot interferometer, while plates reflectivity R is given by the Fabry-Perot interferometer producer.

The minimization of χ^2 merit function must be proceed iteratively, because of nonlinear dependence of model function on fitting parameters. Therefore, Marquardt-Levenberg algorithm is used to optimize values of adjustable parameters during iterations. This algorithm is approved in practice and has became the standard of nonlinear least-square routine (Press et al., 1988). The applied iterative procedure is repeated until χ^2 value stops to decrease, fulfilling the condition that $\Delta\chi^2$ is less then initially entered best-fit value.

The estimated error in determination of adjustable parameters best-fit values is less then several percent.

As an illustration of application of described method, the deconvolution result for neutral atom neon line λ=585.25 nm (natural isotope mixture) is given in Fig.1.

One can see that the overall profile obtained by this method is in agreement with experimental one. In addition, the gas kinetic temperature of a hollow cathode discharge ($T_g=590K$), which is derived from reduced Gaussian halfwidth $\Delta\lambda_D$, corresponds to that one measured by thermocouple (Bukvić, 1984).

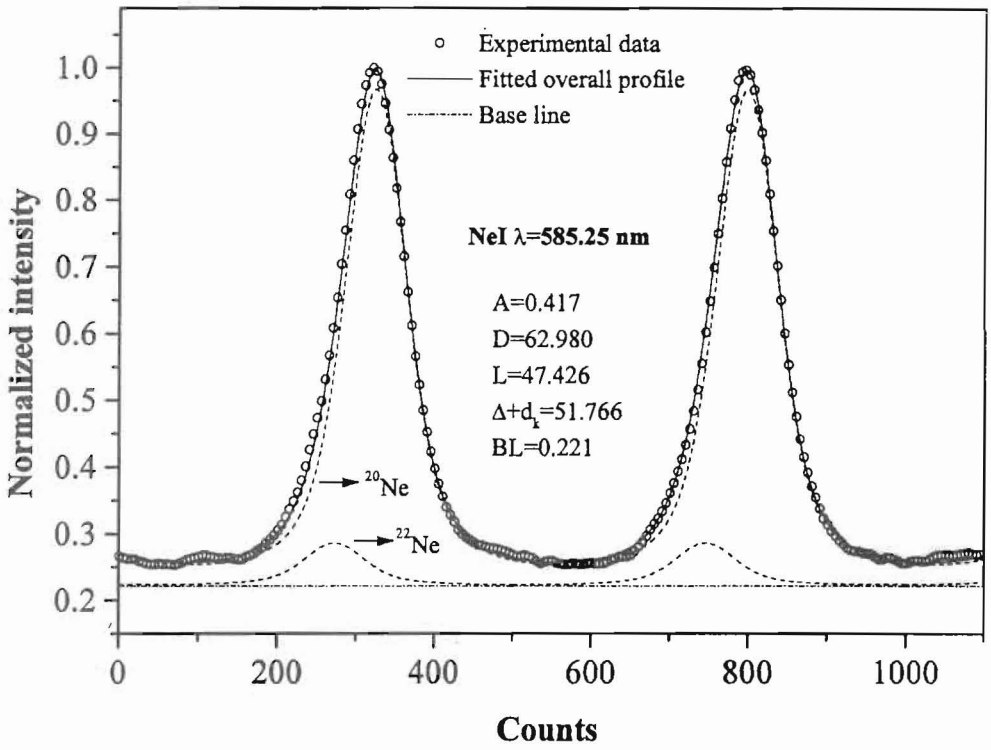

Fig. 1. An example of the deconvolution of atomic neon (natural mixture) spectral line λ=585.25 nm interferogram. The Fabry-Perot interferometer parameters: R=0.985; $\Delta\lambda_s$=473 counts (1count=$36*10^{-15}$ nm).

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