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Validity of the deconvolution method for multicomponent spectral lines

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Abstract. In this paper, we present a study of the validation of the deconvolution procedure for multicomponent overlapping spectral line profiles. The solution of the ill-posed inverse task was implemented using the Tikhonov regularization algorithm. For this study, both, theoretically modelled and experimentally measured 253.7 nm mercury spectral line profiles were used, emitted from high-frequency electrodeless lamps.

1. Introduction

It is well known that the neglecting the instrumental function gives a huge error in the estimation of the discharge temperature from the broadening of the spectral line shapes [1]. It is especially important when the broadening of an instrumental function is on the same order as the experimental profile. In a previous work, a method of spectral line shape modelling was developed for the determination of the real spectral line shape [2]. However, for the use of this method, a lot of *a priori* information about the discharge plasma is necessary. The idea is to develop a robust and simple method for the calculation of the real spectral line shapes. In a previous study, the use of a regularisation method, based on the Tikhonov regularisation principle, was demonstrated for the case of two overlapping spectral lines [3,4]. In this work, this model is validated for multicomponent overlapping spectral lines with the example of a synthesised spectral line and an experimentally measured Hg 253.7 nm line.

2. Validation

An experimentally measured spectral line (*f(v)*) is a convolution of the real line shape(*y(v')*) with an instrumental function (*A(v,v')*). It can be described by the Fredholm first-kind integral equation [5]**:**

$$\int_a^b A(v,v^{'})y(v^{'})dv^{'} = f(v), \quad c \le v \le d, \tag{1}$$

where: a, b and c, d are the limits of the real and measured (experimental) profiles, respectively. The deconvolution procedure is implemented by means of the ill-posed inverse task solution, based on Tikhonov regularization [6]. According to this method, the initial ill-posed task is transformed into a well-posed problem that can be solved by classical methods [4,5,7]. The only *a priory* information required for this calculation is the instrumental function.

For validation of this technique in the case of multicomponent profiles, spectral line shapes of the mercury 253.7 nm line were generated.

Self-absorbed Voigt profiles were simulated by convolution of the Doppler profiles, with full width half maximum (FWHM) $\delta\nu_D$=0.04 cm^{-1}, and Lorentz profiles, with the FWHM $\delta\nu_L$=0.001cm^{-1}. Then synthetic spectra of low-temperature discharge plasmas were simulated using the model described in [3] with the optical density at the line centre k_0l= 5 and the homogeneity of the light source n=13. The simulated real profile was convoluted with the instrument function of a Fabry-Perot interferometer with 3 different coefficients of reflection of the mirrors R = 75%, 85%, and 95%. The instrument function of the Fabry-Perot interferometer is assumed to be an Airy function [2]. The interferometer is characterized also by the free spectral range $\Delta\sigma=1/2t$, where t is the distance between the mirrors [2]. The free spectral range for this model experiment was assumed to be 1.25 cm^{-1}. The deconvolution procedure of the synthesised profiles was implemented and modelled "real" profiles were compared with "real" profiles obtained by the solution.

3. Results and discussion
In figure 1(a,b) and figure 2(a) the comparisons between modelled "experimental", modelled "real" and "real, obtained from solution" profiles are shown. The modelled "experimental" profiles were generated with reflection coefficients R = 75%, 85%, and 95% respectively.
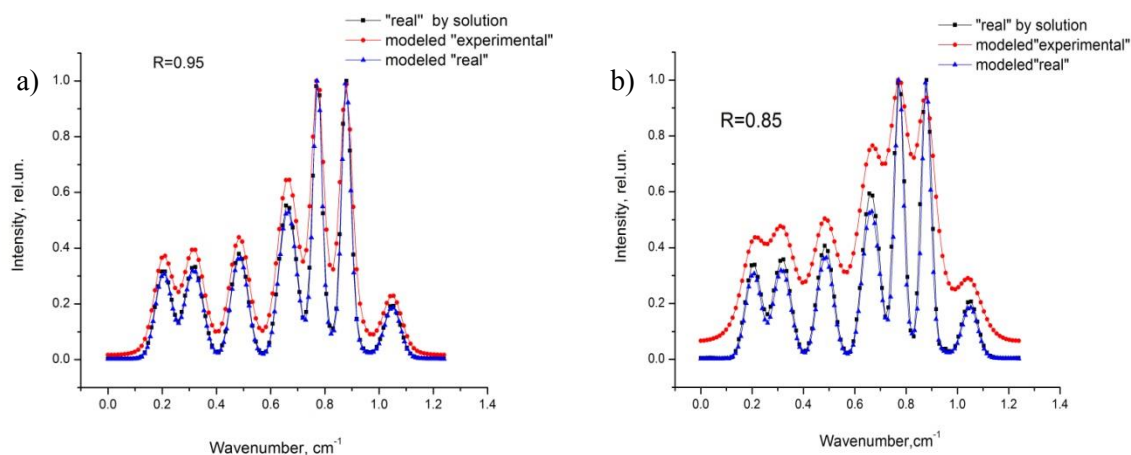

Figure 1. Comparison between the modelled "real" profile, "real by solution" profile and modelled "experimental" profile. The instrumental function is the Airy function with reflection coefficients (a) R = 95%; (b) R = 85%.

Figure 2 (b) shows an example of the results of the deconvolution from an experimentally measured Hg 253.7 nm line profile. The spectral line shapes were measured by means of the Fourier Transform Spectrometer Bruker IFS 125HR [8]. The instrumental function was approximated by a Lorenz function. The regularisation parameter was obtained by two independent methods [2].

As seen in figures 1 and 2, the profiles, modeled and obtained from solution, compare quite well. For the quantitative characterization of agreement between modeled "real" and "real, obtained by solution" we used two statistical methods (see table 2). According to the nonparametric analysis, the two distribution (values, obtained by the means of both methods) are not significantly different (p(probability)>0.05) [9]. The Spearman's correlation coefficients show the significant correlation (p≤0.1) between values, obtained by both methods also [9].
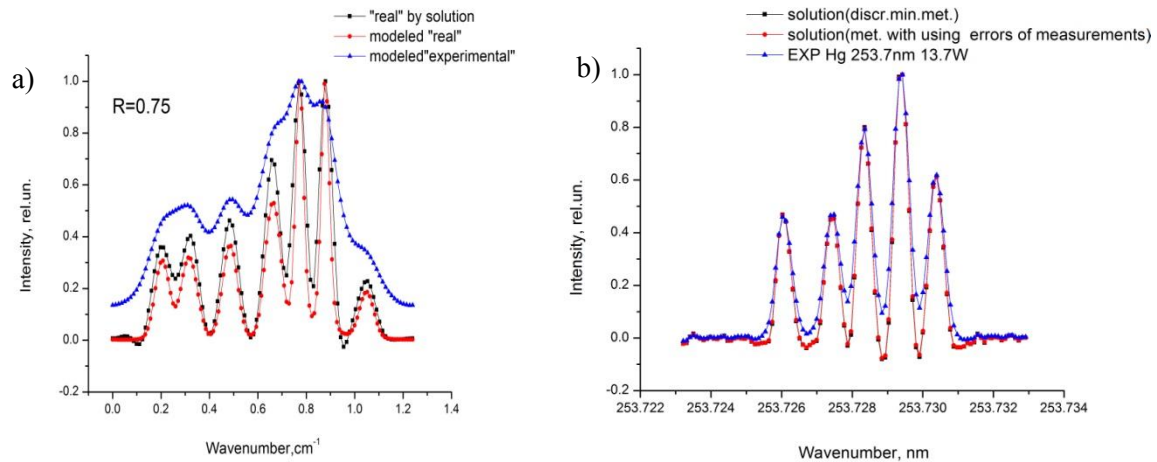
Figure 2. A comparison between (a) modelled "real" profile, "real by solution" profile and modelled "experimental" profile. The instrumental function is an Airy function with R= 0.75; (b) the measured Hg 253.7 nm line and the deconvoluted profile by means of the regularisation.

Table 1. Statistical results

Reflection coeficient	0.95		0.85		0.75	
Number of components	1	9	1	9	1	9
Spearman correlation coef.	0.29	0.34	0.26	0.33	0.23	0.31
p-value	0.004	0.000	0.008	0.001	0.021	0.001
Nonparametric Analysis (Two Sample)						
p-value(Mann-Whitney test)	0.377	0.495	0.286	0.803	0.229	0.502
p-value(Kolmogov-Smirnov test)	0.739	0.622	0.310	0.622	0.310	0.174

4. Conclusions

In this paper, the results of a validation of a method of deconvolution based on Tikhonov regularization method for multicomponent overlapping spectral lines is shown. The Hg 253.7 nm multicomponent spectral line was generated as a convolution of the modelled real self-absorbed Voigt profile with the instrumental function. Spearman's correlation coefficients were obtained, and nonparametric analysis was implemented for the analysis of the agreement between the solutions and modelled real lines.

Acknowledgements

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