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Review paper

EXPERIMENTAL DIFFICULTIES IN DETERMINATION OF THE SPECTRAL LINE SHAPES EMITTED FROM PLASMA*

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SUMMARY: From the plasma radiation and from spectral line profiles it is possible to obtain many particulars about the plasma conditions. The particulars are, for example, concentration of the neutral or charged particles, their temperatures and atomic data. Experimentaly obtained data have great importance in plasma diagnostic, theory testing and plasma applications.

During the experimental work many difficulties appear. The aim of this paper is to classify experimental problems and to offer a method for their solving.

In this paper first a rewiew of spectral line broadening causes and corresponding theories is given. The experimental technique and checking and corrections of self absorption are described also. Furthermore, procedure of spectral line halfwidth and shift determination from experimental profiles is given. Finally, the Abel inversion, important for plasma sources with cylindrical symmetry is considered. All of above mentioned techniques and procedures are followed by many experimental examples.

1. INTRODUCTION

Continuous radiation and spectral line profiles provide a lot of information about the plasma conditions, such as concentration of neutral and charged particles and their temperatures. Experimentally obtained data are of great importance for plasma diagnostics, theory testing, and the different plasma applications.

The passage of radiation through a spectral apparatus results in a radiation spectrum. Onto the continuous part of the spectrum originating from recombination and bremsstrahlung is superimposed the line spectrum resulting from the electron transition within the emitter atom. Spectral lines have always certain profiles, i.e. a definite distribution of the radiation intensities in a given range of wavelengths (frequencies), and therefore, has a finite width. The line shape and width depend upon the type of emitter and the physical conditions under which the emitter is operating, as well as of characteristics of the spectral apparatus employed. The line width is measured at the half of the maximum line height (half-width).

In recording of spectral lines and their treatment, numerous difficulties arise. This work is an attempt to systematize these problems and offer the appropriate solutions.

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The paper provides first a survey of the causes of spectral line broadening, together with short theories describing this phenomenon. The next section is devoted to the experimental techniques of profile recording and treatment of experimental profiles, i.e. the determination of half-widths and shifts of spectral lines. Two separate sections are devoted to experimental techniques of checking and corrections for self-absorption and to the Abel inversion, important for plasma sources with a cylindrical symmetry. Finally a detailed description is given of the procedures for separating particular components of experimental line broadening. All these techniques and procedures are illustrated with a number of experimental examples.

2. SPECTRAL LINE BROADENING

The broadening mechanisms of spectral lines of atoms and ions in plasma can be divided in three groups: a) Natural broadening, caused by finite average lifetime of atoms in excited state, b) Doppler broadening, due to the motion of the emitter atoms with respect to the observation system, and c) Pressure broadening, caused by the interaction of the emitter with the neutral and charged particles.

2.1 Natural broadening

From the point of view of quantum mechanics, the natural line width is a consequence of the energy uncertainty of stationary atomic states. This uncertainty is given by the well known Heisenberg relation stating that the uncertainty of energy of the excited state is inversely proportional to the atom lifetime τ_n in this state:

$$\Delta E \simeq \frac{h}{2\,\pi\,\tau_n} \tag{2.1.1}$$

In this case, the line half-width is:

$$\Delta\nu \approx \frac{1}{2\,\pi}\left(\frac{1}{\tau_n}+\frac{1}{\tau_m}\right) \tag{2.1.2}$$

The radiation distribution with respect to frequencies (wavelengths) is symmetrical, and is given by the Lorentz distribution (Mitchner and Kruger, 1973). It is evident from (2.1.2) that the natural half-width is proportional to the sum of transition probabilities $(1/\tau)$. As the transition probabilities are very different for various transitions, the natural half-width for various transitions will be different. For plasma-emitted spectral lines, natural broadening is in the majority of cases negligible.

2.2 Doppler broadening

Excited atoms and ions as the radiation sources in plasma are in the state of constant motion. This can be thermal motion, motion due to turbulence, or the motion of either the plasma as a whole or its part with respect to the observer. Thus, the Doppler effect arises, which means that the observer measures higher frequencies (shorter wavelengths) of the approaching source, and vice versa. The distribution of radiation intensities against the wavelengths due to the Doppler effect is of the Gaussian type (Frish, 1963). The Doppler line half-width is calculated as:

$$\Delta\lambda = 7.162\times10^{-7}\,\lambda_0\left(\frac{T}{M}\right)^{1/2} \tag{2.2.1}$$

where T is expressed in K and M in atomic mass units.

2.3 Pressure broadening

Broadening of spectral lines caused by the interaction of the emitter with the surrounding particles (perturbers), depends on the concentration of these particles, and is called pressure broadenining. Depending on the type of interaction of the emitter and perturber this broadening may be either: a) Resonance broadening, if the emitter interacts with the perturber of the same type, b) Van der Waals broadening, if the interaction with neutral particles is involved, or c) Stark broadening, when the perturbers are charged particles, electrons and ions. Under real conditions, these broadening mechanisms act simultaneously.

Resonance broadening

Resonance broadening appears when either the upper or the lower level of the observed transition has the allowed dipol transition to the ground state, and when the emitter is surrounded by similar atoms in the ground state. If we consider two identical atoms, then it is unimportant which of the atoms is excited and which is in its ground state. In this case the considered level is degenerated, and the final result is the spectral line broadening. This process may also be considered as the shortening of the duration of the excited state due to the energy exchange, so that a broadened spectral line is observed. Starting from the theories of Baranger (1962) and Griem et al. (1962), Griem (1964) derived an expression for the spectral line width due to the dipol-dipol interaction with the ground level of the same sort of atoms. Later, Ali and Griem (1965; 1966) corrected this expression and obtained the following equation for the half-halfwidth due to resonance broadening:

$$\omega_R = 1.92\,\pi \left(\frac{g_1}{g_R}\right)^{1/2} \frac{N\,e^2\,f_R}{m\,\omega'} \tag{2.3.1}$$

where g_1 and g_R are the statistical weights of the ground and excited level, N concentration of the perturbed particles, f_R the oscillator strength, m the electron mass and ω' the corresponding angular frequency. Resonance broadening may be caused by atoms and ions of another kind provided their energy levels are close to the corresponding atomic level of the emitter. In terms of wavelengths, the above expression for the resonance half-halfwidth assumes the form:

$$\mathrm{w}_R = 4.30 \times 10^{-14} \left(\frac{g_1}{g_R}\right)^{1/2} \lambda^2\,\lambda_R\,f_R\,N \tag{2.3.2}$$

where λ is the wavelength of the considered radiation in (cm), and λ_R is the wavelength of the resonance transition.

Van der Waals broadening

The forces by which neutral atoms are acting on the atom-emitter are of short-range type. The position of the considered level of the emitter atom depends on the emitter-perturber distance. Averaging over all the possible distances between the emitters and neutral perturbers results in broadening of the resulting spectral lines. The intensity maximum of the line will be shifted in comparison to the radiation of the unperturbed atom, and it will appear at the wavelength corresponding to the most probable distance between the emitter and perturber.

Griem (1964) estimated the van der Waals half-halfwidth, which may be written in the following form (Kelleher, 1981):

$$\omega_V = \pi \left(\frac{4\,\pi}{3}\right)^{4/5} C^{2/5}\,\overline{v}^{3/5}\,N \tag{2.3.3}$$

where $\bar{v}$ is the average relative velocity of colliding atoms, N the puterber concentration, and C is the difference of the van der Waals constants for the upper and lower level:

$$C = C_i - C_f \tag{2.3.4}$$

where:

$$C_i = \overline{\alpha}\,\frac{e^2\,a_0^2}{h}\,\overline{R_i^2} \tag{2.3.5}$$

The quantity $\overline{\alpha}$ is the average polarizability of neutral perturbers, expressed as (Griem, 1964; Allen, 1973):

$$\overline{\alpha} = \frac{9}{2}\,a_0^3 \left(\frac{3\,E_H}{4\,E_{2p}}\right)^2 \tag{2.3.6}$$

where a_0 is the Bohr radius, E_H the ionization energy of hydrogen atom, E_{2p} the energy of first excitation level of the perturber. In (2.3.5) $\overline{R_i^2}$ denotes the square of the position vector of the excited electron, which in a Coulombic approximation is:

$$\overline{R_i^2} = \frac{n_i^{*2}}{2}\left[5\,n_i^{*2} + 1 - 3\,l_i\,(l_i+1)\right] \tag{2.3.7}$$

where l_i is the corresponding orbital quantum number, and n_i^* the effective quantum number:

$$n_i^* = \left(\frac{E_H}{E_J - E_i}\right)^{1/2} \tag{2.3.8}$$

and E_J is the emitter's ionization energy, and E_i the energy of the considred level of the emitter atom. In terms of wavelengths, the van der Waals half-halfwidth can be expressed as (Kelleher, 1981):

$$\mathrm{w}_V = 4.09 \times 10^{-12}\,\lambda^2 \left(\overline{\alpha}\,\overline{R^2}\right)^{2/5} \left(\frac{T}{\mu}\right)^{3/10} N \tag{2.3.9}$$

where μ is the reduced mass of the emitter-perturber system, and $\overline{R^2}$ is:

$$\overline{R^2} = \overline{R_i^2} - \overline{R_f^2} \tag{2.3.10}$$

The van der Waals broadening is significant only for the plasmas with high concentration of neutral particles.

Stark broadening

The Stark broadening is observed as a change in atomic energy levels positions under the action of electric field. In plasma, this is the electric microfield created by the charged particles, electrons and ions. The radiation of particular atoms consists of the lines shifted and splitted into components, but in contrast to a static electric field, the electric microfield in plasma is changing in space and time, and these changes are different for the various atoms, so that the net effect is the spectral lines which are broadened and shifted.

For the hydrogen atom and hydrogen-like ions is characteristical so-called linear Stark effect. Namely, the amount of energy by which a given energy level of an atom in the electric field is shifted is proportional to the strength of this field.

In the case of "non-hydrogenic" atoms there is a quadratic dependence between the additional energy and electric field intensity, that is the quadratic Stark effect is involved. After the appearance of the works of Baranger (1958, 1958, 1958) and Kolb and Griem (1958), the Stark broadening of spectral lines has become a subject of numerous theoretical papers.

In the present work we are not going to deal with the classification and analysis of these works, as there are several monographs and review articles

devoted to the Stark broadening of spectral lines (Baranger, 1962; Griem, 1964, 1974, 1975; Breene, 1964; Sobelman, 1972; Lisica, 1977), as well as critical reviews of experimental data (Konjenić and Roberts, 1976; Konjević and Wiese, 1976, 1990; Konjević et al., 1984, 1984). The bibliography concerning the problem of spectral line broadening has been prepared by Fuhr et al. (1972, 1974, 1975, 1993).

The ions and electrons, as perturbers, can be treated separately because of large differencies in their masses and velocities in interactions with atoms and ions as emiters. Starting from this assumption, two approximations in the theories of Stark broadening have been adopted: quasi-static (ion) and impact (electron) approximation. The impact approximation (Griem, 1974) gives as a result a symmetrical Lorentz form spectral line:

$$I(\omega) = \frac{\mathrm{w}_e}{\pi} \frac{I_0}{(\omega - \omega_0 - d)^2 + \mathrm{w}_e^2} \tag{2.3.11}$$

with a half-width w_e and shift d_e determined by the following expressions:

$$\begin{aligned} \mathrm{w}_e &= -\frac{1}{\hbar} I_m \; ' \, if^* \mid H \mid if^* \gg = \\ &= -R_e \; ' \, if^* \mid \Phi \mid if^* \gg \end{aligned} \tag{2.3.12}$$

$$\begin{aligned} d_e &= \frac{1}{\hbar} R_e \; ' \, if^* \mid H \mid if^* \gg = \\ &= -I_m \; ' \, if^* \mid \Phi \mid if^* \gg \end{aligned} \tag{2.3.13}$$

These expressions represent fundamental results of the impact approximation, on the basis of which, using different theoretical approaches (as for example in Griem et al., 1962; Cooper and Oertel, 1967, 1969), one can obtain the parameters w_e and d_e, determining the Lorentz shape and shift of the spectral line.

2.4 Effect of ions on broadening of isolated lines

In acting as perturbing particles, ions are usually less effective in spectral line broadening than electrons. The exceptions are the lines belonging to one-electron systems and the lines with forbidden components, though in these cases ion broadening is not dominant. Because of this, in considering the isolated line profiles the ion broadening is calculated as a small correction for the electron impact broadening. Calculation of this type of line profile, the so-called $j(x)$ profile, in quasi-static approximation, Griem et al. (1962) and Griem (1964), can be written in the form:

$$j_{A,R}(x) = \frac{1}{\pi} \int_0^\infty \frac{W_R(\beta) \; d\beta}{1 + (x - A^{4/3} \, \beta^2)^2} \tag{2.4.1}$$

where $W_R(\beta)$ is the electric micro-field distribution, β is the ratio of the electric field and Holtsmark field strength (F/F_0), and x is the reduced frequency, or the reduced wavelength:

$$x = \frac{\omega - \omega_0 - d}{\mathrm{w}_e} = \frac{\lambda - \lambda_0 - d}{\mathrm{w}_e} \tag{2.4.2}$$

where ω_0 is the unperturbed frequency, and w_e and d_e are impact half-halfwidth and shift, respectively. Expression (2.4.1) is also dependent on two additional parameters, the ion-broadening parameter A, and the Debye shielding parameter R:

$$A = \left(\frac{C \, F_0^2}{\mathrm{w}_e} \right)^{3/4} \tag{2.4.3}$$

$$R = 6^{1/3} \, \pi^{1/6} \left(\frac{e^2}{k \, T} \right)^{1/2} N^{1/6} \tag{2.4.4}$$

where $C = C_4/e$ and C_4 is the constant of the quadratic Stark effect. The profile $j_{A,R}(x)$ with the ion effect taken into account, gives the additional shift and line asymmetry. Expressions for the half-width and shift of the maximum of the line, described by the $j_{A,R}(x)$ profile, can be written in the form (Konjević and Roberts, (1976):

$$\begin{aligned} \mathrm{w}_{stat} \simeq 2 \, \mathrm{w}_e \Big[& 1 + 1.75 \times 10^{-4} \, N_e^{1/4} \, A \\ & \left(1 - 0.068 \, N_e^{1/6} \, T^{-1/2} \right) \Big] \; 10^{-16} \, N_e \end{aligned} \tag{2.4.5}$$

$$\begin{aligned} d_{stat} \simeq \Big[& d_e \pm 2.00 \times 10^{-4} \, N_e^{1/4} \, A \, \mathrm{w}_e \\ & \left(1 - 0.068 \, N_e^{1/6} \, T^{-1/2} \right) \Big] \; 10^{-16} \, N_e \end{aligned} \tag{2.4.6}$$

where the values of parameters w_e, d_e and A are taken for the electron concentration of $N = 1 \times 10^{16} cm^{-3}$, as it was given in Griem (1974).

Because of the asymmetry of the line profile, the shift measured at the half of line height $d_{stat1/2}$ differs from that measured for the maximum. This difference can be expressed by different numerical coefficients in the second term of (2.4.6) (Kelleher, 1981):

$$\begin{aligned} d_{stat1/2} \simeq \Big[& d_e \pm 3.20 \times 10^{-4} \, N_e^{1/4} \, A \, \mathrm{w}_e \\ & \left(1 - 0.068 \, N_e^{1/6} \, T^{-1/2} \right) \Big] \; 10^{-16} \, N_e \end{aligned} \tag{2.4.7}$$

The sign before the second term in the shift expressions (2.4.6) and (2.4.7) is determined by the sign of the electron impact shift d_e in the range of low temperatures.

The application of the above expressions for the half-width and shift of spectral lines of neutral atoms is limited by the conditions $R \leq 0.8$ and $0.05 \leq A \leq 0.5$. For the values $A \leq 0.05$, in considering the emitter-perturber interactions, one has to take also into account the quadrupole effect. The values

$A \geq 0.5$ correspond to the conditions when the linear Stark effect is predominant. In the case $A \leq 0.05$, the line half-width is calculated in the following way (Griem, 1974):

$$\mathrm{w}_{stat} = 2\,\left(\mathrm{w}_e\, N_e \times 10^{-16} + \mathrm{w}_i\right) \tag{2.4.8}$$

where:

$$\mathrm{w}_i = 2\,\pi\, N\, \frac{(n_i^{*2} - n_f^{2*})^2}{Z^2\, m}\, \hbar\, a_0\, Z_p \tag{2.4.9}$$

N denotes the perturber concentration, a_0 is the Bohr radius, m the electron mass, n_i^* and n_f^* the effective quantum numbers of the initial and final state, respectively (eq. (2.3.8)), Z has the value 1 for neutral atoms, 2 for singly-charge atoms, etc., and Z_p is the multiplicity of the perturber charge. The half-width obtained from (2.4.8) is compared to that obtained from (2.4.5), and the larger of the two values is taken as the result.

In some cases, especially when light ions are considered, the ion motion cannot be neglected, as it has been done in the quasi-static approximation. There are two theoretical approaches (Griem, 1974 and Barnard et al., 1974) for evaluation of the fluence of ion dynamics to the width and shift. The correspondence between the quantities used by two mentioned theories is given in Kelleher (1981). Dimitrijević and Sahal-Brechot (1990) also included ion dynamics effects in their theoretical calculations.

The half-width and shift at the half-height can be expressed in the form (Barnard et al., 1974) similar to (2.4.5) and (2.4.7):

$$\mathrm{w}_{dyn} \simeq 2\,\mathrm{w}_e\, \left[1 + 1.75 \times 10^{-4}\, N_e^{1/4}\, A\, W_j \left(1 - 0.068\, N_e^{1/6}\, T^{-1/2}\right)\right]\, 10^{-16}\, N_e \tag{2.4.10}$$

$$d_{dyn1/2} \simeq \left[d_e \pm 3.20 \times 10^{-4}\, N_e^{1/4}\, A\, \mathrm{w}_e\, D_j \left(1 - 0.068\, N_e^{1/6}\, T^{-1/2}\right)\right]\, 10^{-16}\, N_e \tag{2.4.11}$$

These expressions differ only in the additional coefficents W_j and D_j, which can be expressed as (Kelleher, 1981; Kobilarov, 1989):

$$W_j = \begin{cases} 1.36\, B^{-1/3}/g & ,\ B < (1.36/g)^3 \\ 1 & ,\ B \geq (1.36/g)^3 \end{cases} \tag{2.4.12}$$

$$D_j = \begin{cases} 1.75\,[2.35\, B^{-1/3} - \\ 3\,(10^{-4}\, A\, N_e^{1/4})^{1/3}\, R]/2\, g & ,\ B < 1 \\ 1 & ,\ B \geq 1 \end{cases} . \tag{2.4.13}$$

where:

$$B = \frac{0.0806\,\mathrm{w}_e}{\lambda^2}\, \left(\frac{\mu}{T}\right)^{1/2}\, \left(10^{-4}\, A\right)^{1/3}\, N_e^{3/4} \tag{2.4.14}$$

T_g is the gas temperature, μ is the reduced mass calculated from the mass of the emitter m_{em} and perturber m_p as:

$$\frac{1}{\mu} = \frac{1}{m_{em}} + \frac{1}{m_p} \tag{2.4.15}$$

and

$$g = 1.75\,(1 - 0.75\, R) \tag{2.4.16}$$

As can be seen from these expressions, the parameters W_j and D_j are dependent of the electron temperature, gas temperature, electron concentration, and the reduced emitter-perturber mass. For $W_j = 1$ and $D_j = 1$, the effect of ion dynamics is negligible, and quasi-static approximation can be used ((2.4.5), (2.4.6) and (2.4.7)).

3. EXPERIMENTAL SETUP FOR SPECTRAL LINE PROFILES RECORDING

Typical experimental setup for recording profiles and shifts of spectral lines is presented in Fig. 3.1. Usually, the plasma image is projected with the aid of the mirror system (M_1, M_2) onto the entrance slit of the monochromator at the ratio 1:1. The choice of the appropriate spheric mirror M_2 and its position with respect to the plasma source and monochromator should ensure total irradiation of the dispersion grating of the monochromator. Optical alignment of the system plasma source - mirror - monochromator is carried out with the aid of the He-Ne laser. The radiation coming from the plasma source passes also through the partly transparent (reflecting) mirror M_3. This enables observation of the radiation from the reference source, used for spectral line shift measurements. After its amplification with the aid of a photomultiplier placed after the monochromator, the signal is led to the appropriate instrument. The most suitable for this purpose is a digital oscilloscope, irrespective of whether we deal with a pulse or continuous plasma source, as digital oscilloscope has the capability of signal averaging. In the case of a pulse source, a large number of signals may be averaged, whereas in the case of a continuous plasma source the averaging is carried out over time. In this way, a favourable signal-to-noise ratio is achieved and the measurement error is lowered.

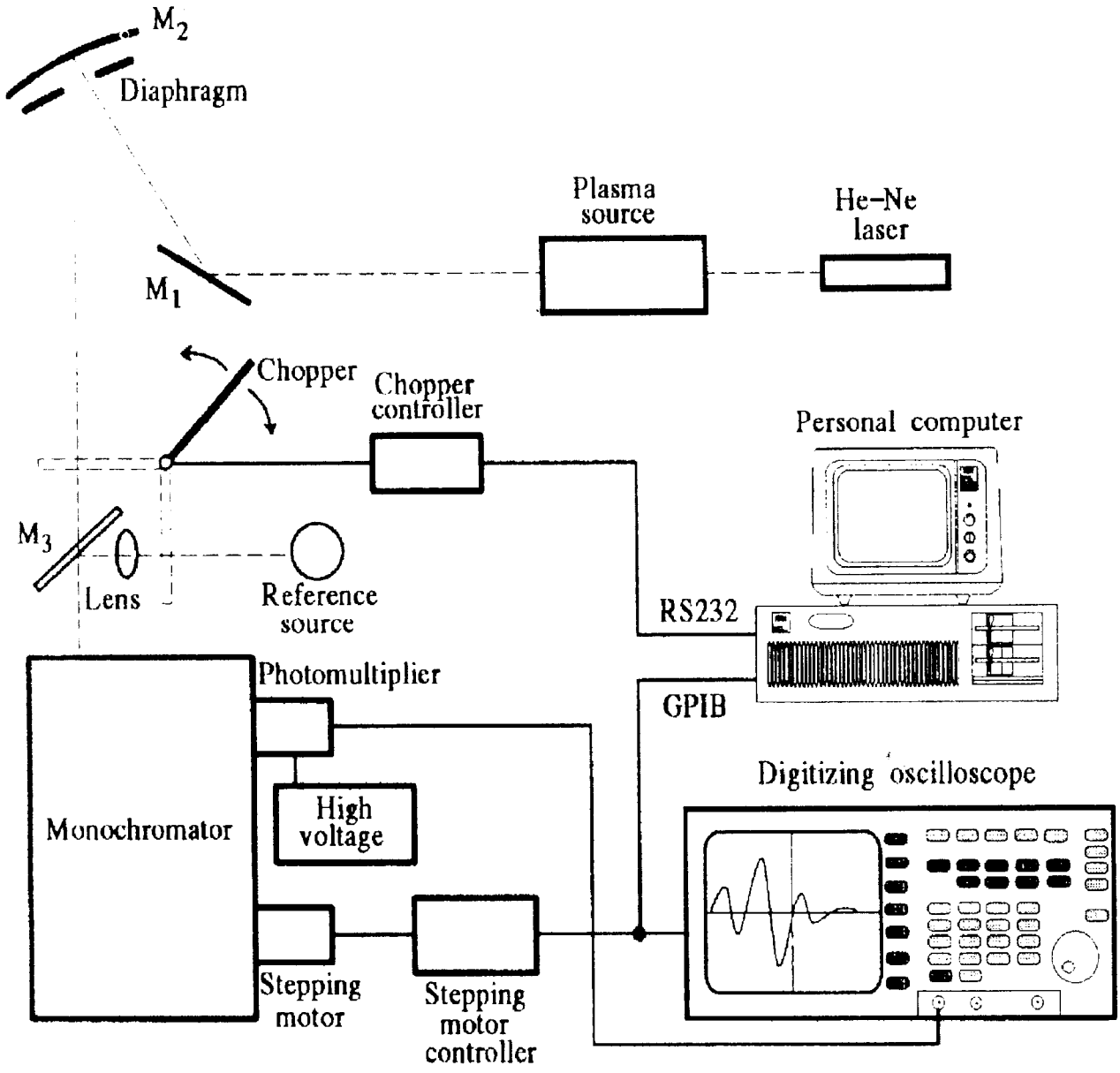

Fig. 3.1 Schematic diagram of the experimental setup.

Besides, of special importance is the possibility of computer control and acquisition of measurement data during the experiment. This normally decreases the possibility of making mistakes, which is the case when a large number of parameters are changed and registered manually during the tedious process of recording of spectral line profiles. Generally, the error of measuring spectral line parameters using digital oscilloscope and computer-controlled experiment is below 5%, which represents a substantial advantage over the classical experiment, in which the error is typically in the range of 15-30%.

Spectral line profile is obtained by scanning the radiation intensity in a given range of wavelengths. This enables measurement of the half-width of the experimental profile of the considered spectral line. To measure spectral line shift we need a reference source of radiation. Reference radiation sources are usually those working at a low pressure, such as the Geissler tube, hollow cathode, or high-frequency discharge. The reference source should emit the same line, or a line which is quite close to the considered line of the plasma source. As the reference radiation source operates at a low pressure, the emitted lines are not shifted, and are only naturally broadened. This enables measurement of the spectral line shift by simply comparing the position of the source line to that of the reference line. With the aid of mirror M_3, it is possible to ensure simultaneous observation of the radiation from the plasma source and reference source. The experimental profile thus obtained and registered on a strip-chart recorder (Djurović et al., 1988) is presented in Fig. 3.2. In this case it is necessary to carry out separation of profiles, as the resulting profile of simultaneous recording contains both the observed and the reference line. A much better solution is to use a light chopper (Fig. 3.1). In that case at a given wavelength is recorded the signal, for example, from the plasma source, and then

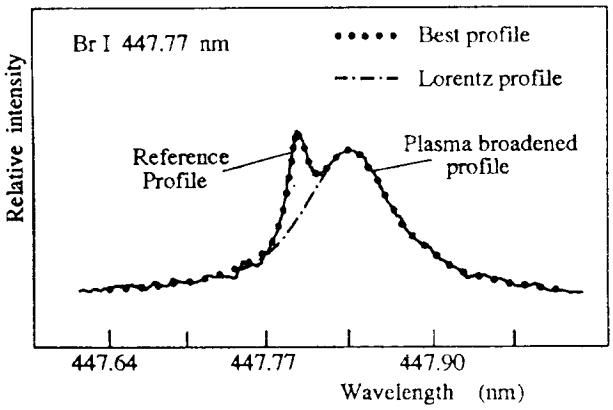

Fig. 3.2 Example of the shift measurement (strip chart recording).

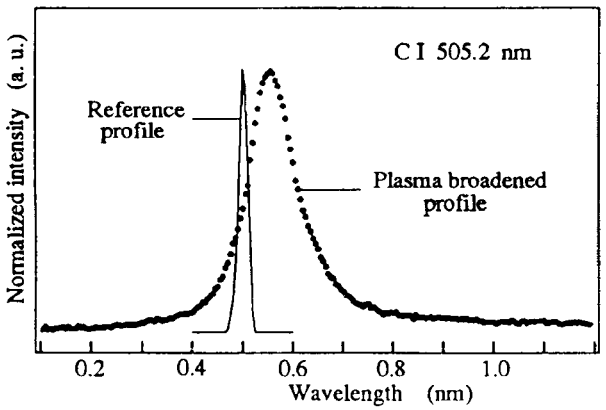

Fig. 3.3 Example of the shift measurement (digital oscilloscope recording).

the signal coming from the reference source, after which the wavelength is changed and the procedure repeated. The profiles thus obtained are presented in Fig. 3.3 (Mijatović et al., 1995).

In addition to shift measurements, the profile of spectral line from the reference source may also be used for determining the instrumental broadening. Namely, because of the absence of other causes of line broadening except the natural one, which is negligible, the half-width of the reference source profile is at the same time the instrumental half-width. The instrumental profile of a spectral line may be very well described by a Gaussian profile. An example of such profile is given in Fig. 3.4.

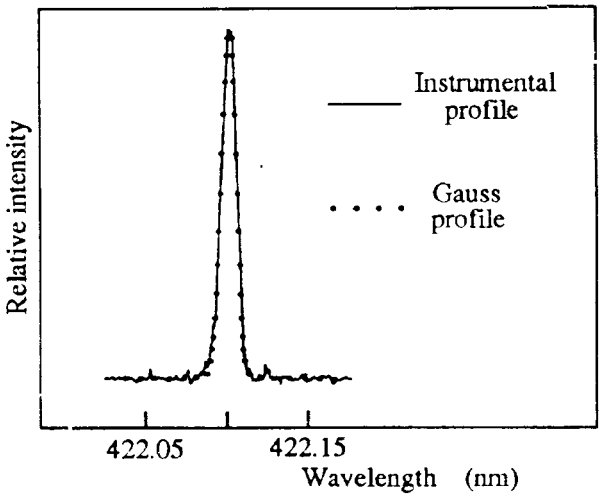

Fig. 3.4 Example of instrumentally broadened profile.

Experimental profiles of the given spectral lines may be the basis for testing the conditions of local thermodynamic equilibrium and thus enable the plasma diagnostics, i.e. the determination of electron concentration and temperature, as well as of some other parameters. However, this is not going to be the subject of our present concern, and the further text will be confined only to the treatment of experimental profiles.

4. SELF-ABSORPTION OF SPECTRAL LINES IN PLASMA

Before any treatment of the experimental profile it is necessary to check the self-absorption of spectral lines, and then eliminate its causes, or correct the experimental profile. The self-absorption corrections are possible only when influence of cold plasma layers is negligible. Such a cold plasma layer, in which exists a high gradient of electron concentration and temperature, is, for example, the plasma layer near to the electrode or to vessel wall. In cases when influence of cold plasma layer is not negligible, the passage of radiation through a cold layer may result in a distorted experimental spectral line profile and large error may be made in line parameters determination.

There are several ways for testing the existence and eliminating the origin or the effect of self-absorption. Which of these methods will be applied depends on experimental conditions and plasma source, as well as on the spatial distribution of emitter particles within the plasma source.

In the cases the atomic systems can be described by the LS coupling, the existence of self-absorption can be checked in a simple way (Konjević and Wiese, 1976). Namely, in some case of LS coupling the ratios of spectral lines intensities are well known (Lindholm, 1941; Shore and Menzel, 1968). Hence, the procedure of checking the existence of self-absorption is reduced to the comparison of the line intensities within the multiplet. If the ratio of the strongest line and the weaker ones in a multiplet is lowered, then self-absorption is present. For such a comparison it is sufficient to measure intensity of the line maxima.

By decreasing the concentration of emitter particles one can eliminate self-absorption. After lowering the concentration it is possible to check again the intenisties of the multiplet lines. Besides, a check of the existence of self-absorption can also be obtained on the basis of the half-width of a particular spectral line. It is best to use the strongest line in the multiplet, because this line is most sensitive to the self-absorption. If self-absorption is present, a decrease in concentration will result in a decrease in the half-width of the experimental profile. When at a certain concentration there is no change in the line half-width compared to the previous concentration, this means that the conditions are attained under which self-absorption is eliminated. This may not be the best solution in general, as in some cases small concentrations of the emitter give small intensities, so that the measurement error is increased, or the measurement is made almost impossible.

In the case when the element whose lines are of interest is introduced into the central part of plasma of the finite length l, it is possible to carry out not only the self-absorption test but also reconstruct the spectral line profile under the given conditions. This is a very frequent case, for example, with the wall-stabilized electric arcs (Djurovic, 1989). The spherical mirror is placed behind the plasma source at two focal lengths from the plasma centre, as shown in Fig. 4.1a. Between this mirror and the plasma source there is a chopper, so that the optical path between the plasma and the mirror may be either open or closed. In this way at the entrance slit of the monochromator appears alternatively the radiation with or without the radiation reflected from the spherical mirror. An illustration of the profile recorded in this way is presented in Fig. 4.1b. If we denote by I_λ the radiation intensity from the plasma centre, then, after passing through the plasma of the optical thickness $\tau_\lambda = k_\lambda\, l$, the radiation reaching the monochromator entrance slit will be of the following intensity:

$$J_\lambda = I_\lambda\, exp(-k_\lambda\, l) \tag{4.4.1}$$

k_λ being the absorption coefficient, and l is the half of the plasma length. The intensity of reflected radiation reaching the monochromator slit after passing through the whole plasma length may be written as:

$$J^*_\lambda = r\, J_\lambda\, exp\,(-2\, k_\lambda\, l) = r\, I_\lambda\, exp\,(-3\, k_\lambda\, l) \tag{4.4.2}$$

where $rI_\lambda = I^*_\lambda$, and r is the reflection coefficient of the mirror. According to the notation used in Fig. 4.1b we can write:

$$I_\lambda = J_\lambda + \Delta J_\lambda \tag{4.4.3}$$

$$I^*_\lambda = J^*_\lambda + \Delta J^*_\lambda \tag{4.4.4}$$

where ΔJ_λ and ΔJ^*_λ denote the corresponding corrections for self-absorption. The mirror reflection coefficient can be expressed as the ratio of unabsorbed radiation intensities at the wavelength λ in the interval of the spectral line wavelengths, or, as the ratio of radiation intensities in the continuum where there is no absorption:

$$r = \frac{I^*_\lambda}{I_\lambda} = \frac{I^*_C - I_C}{I_C} \tag{4.4.5}$$

On the basis of the above expressions it is possible to calculate the correction of the absorbed profile at the wavelenth λ:

$$\Delta J_\lambda = J_\lambda \left[\left(r\, \frac{J_\lambda}{J^*_\lambda} \right)^{1/2} - 1 \right] \tag{4.4.6}$$

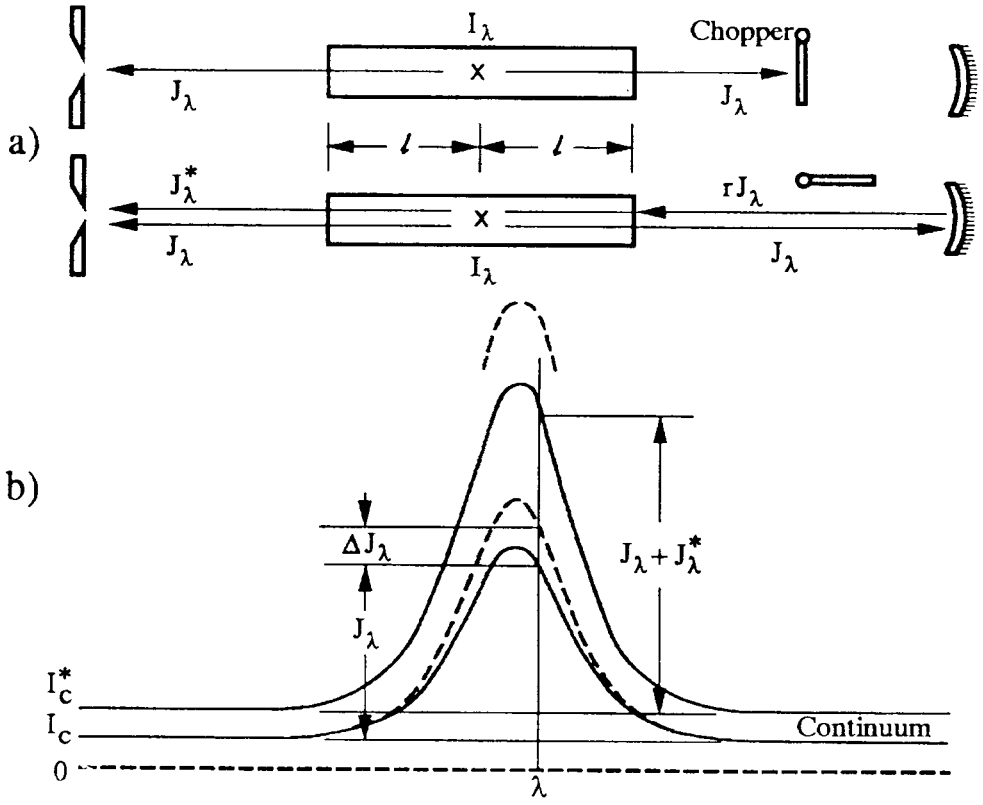

Fig. 4.1 Illustration of checking for self-absorption with concave mirror.

i.e. to obtain the radiation intensity from the plasma centre:

$$I_\lambda = J_\lambda \left(r \frac{J_\lambda}{J^*_\lambda} \right)^{1/2} \tag{4.4.7}$$

The latter expression enables a point-by-point reconstruction of the whole profile of the absorbed line (in Fig. 4.1b this profile is presented by the dotted line). Of course, such a correction can be carried out only if the condition $k_\lambda\, l \leq 1$ is fulfilled. From the above expressions we can calculate:

$$\tau_\lambda = k_\lambda\, l = \frac{1}{2}\, ln \left(r \frac{J_\lambda}{J^*_\lambda} \right) \tag{4.4.8}$$

It suffices to check the condition $k_\lambda\, l \leq 1$ with the aid of (4.4.8) only at the line maximum because the absorption coefficient k_λ has its highest value at the line centre.

In some cases, the self-absorption test and correction of spectral line profile may be done by changing the plasma length (Fig. 4.2). This technique is described in Kobilarov et al. (1989).

According to (4.4.1) we can write:

$$J_{\lambda 1} = I_{\lambda 1}\, exp\,(-k_\lambda\, l_1) \tag{4.4.9}$$

$$J_{\lambda 2} = I_{\lambda 2}\, exp\,(-k_\lambda\, l_2) \tag{4.4.10}$$

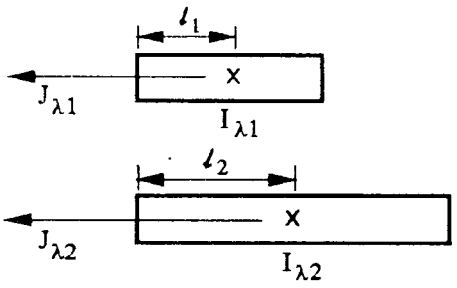

Fig. 4.2 Illustration of checking for self-absorption by changing plasma length.

where the intensity ratio $I_{\lambda 2}/I_{\lambda 1}$ is equal to the ratio of the continuum radiation intensities:

$$\frac{I_{\lambda 2}}{I_{\lambda 1}} = \frac{I_C^*}{I_C} = c \qquad (4.4.11)$$

On the basis of (4.4.9), (4.4.10) and (4.4.11) we can obtain an expression for the absorption coefficient:

$$k_\lambda = \frac{1}{l_2 - l_1}\, ln\left(c\,\frac{J_\lambda}{J_\lambda^*}\right) \qquad (4.4.12)$$

Now, from (4.4.9) or (4.4.10) we can calculate the unabsorbed intensities $I_{\lambda 1}$ or $I_{\lambda 2}$, and thus reconstruct the spectral line profile.

In the case the emitter atoms are homogeneously distributed along the plasma cylinder one should start from the radiation intensity emitted from the plasma of the length l (Wiese, 1965):

$$I_\lambda = B_{\lambda,T}\ [1 - exp\,(-k_\lambda\, l)] \qquad (4.4.13)$$

where $B_{\lambda,T}$ is the Planck function. On the basis of (4.4.13) for two different plasma lengths we can write two equations enabling us to calculate the absorption coefficient after expanding the exponential term and taking into account only a few first-order terms. A change of the plasma length, for example in the pulsed arc or z-pinch, may be carried out in a relatively simple way using an auxiliary electrode in the discharge tube, as described in Kobilarov et al. (1989) and Radtke and Gunter (1986).

5. EXPERIMENTAL PROFILES OF SPECTRAL LINES

Generally, experimental profile of a plasma-emitted spectral line is shifted compared to that which would be emitted by the unperturbed atoms, and is also broadened. The technique of the spectral line shift measurements was discussed earlier in Section 3. All the above mentioned mechanisms of spectral line broadening influence the shape of experimental profile, but their contributions are different.

The experimental profile half-width w_{exp} is usually measured by the procedure illustrated in Fig. 5.1. Of the greatest importance is to determine well the continuum level. In practice, line profiles are usually recorded within a wavelength interval of several half-widths (at least three), on the left and right from the line centre. A better alternative of determining experimental half-width is to fit the experimental profile onto a corresponding theoretical profile.

In the case of predominant Stark effect, the experimental profile of the line due to the emission of neutral atoms may be quite well described by a $j(x)$ profile. For ionic lines the Stark profile is of the Lorentz form. In Fig. 5.2 (Vujičić et al., 1989), the experimental profile of the He I 667.8 nm line is compared to the $j(x)$ profile taken from Griem (1974), where the $j(x)$ profile has been given in a relatively narrow interval (x(-2,+5)). For this purpose it is better to use reference Woltz (1986), providing the $j(x)$ profile in a substantially wider interval (x(-20,+20)), corresponding to about 3.5 half-widths on the left and right from the line maximum. However, when the ion-broadening parameter A is small, i.e. when the profile asymmetry is low, the experimental profile can be described well by the Lorentz profile (Fig. 5.3) (Djurović, (1989). In the case when the Doppler effect has also a significant contribution to the line broadening, which is a frequent case with the laboratory plasmas, the experimental profile is better described using a theoretical profile which is the convolution of the $j(x)$ profile and Gaussian profile. When A is small, one can use the profile which is a convolution of the Lorentz and Gaussian profile, the so-called Voigt profile. The half-width taken for fitting is at the same time the half-width of the experimental profile, w_{exp}.

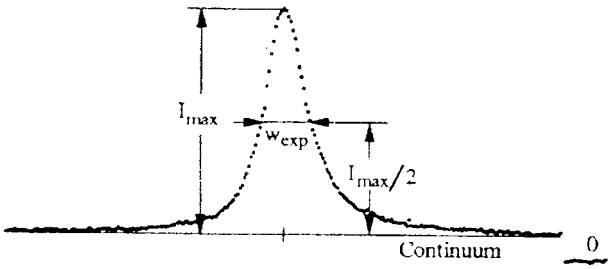

Fig. 5.1 Illustration of half-width measurement.

Up to now we have considered the cases of isolated spectral line profiles. When several close spectral lines whose profiles are overlapping are considered the only way to measure line parameters is to separate these profiles. In Fig. 5.4 is presented an example of lines of neutral chlorine from the multiplet $(^1D)\,4s\,^2D - (^1D)\,4p\,^2D^0$ (Djurović et al., 1990). As the ion-broadening coefficient of these lines is very small ($A \approx 0.02$) the fitting of the recorded part of the spectrum was made using the Lorentz functions. The prescribed parameters (positions, intensities, half-widths) for which best agreement with experimental data was obtained are in fact the parameters of separated profiles presented in Fig. 5.4 by dotted lines.

In Fig. 5.5 is presented another example in which, in addition to measuring of the half-width of the I I 486.23 nm line (Djurović, 1989), the line shift is also measured. The line is superimposed onto the peak of the H_β line which is used for diagnostic purpose. The observed iodine line was fitted by the Lorentz profile, the reference line by the Gaussian profile, whereas the peak of the H_β profile was fitted by two Lorentz profiles.

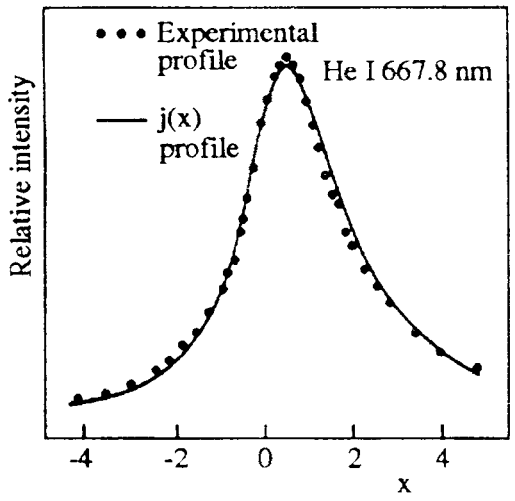

Fig. 5.2 Comparison of experimental and $j(x)$ profile.

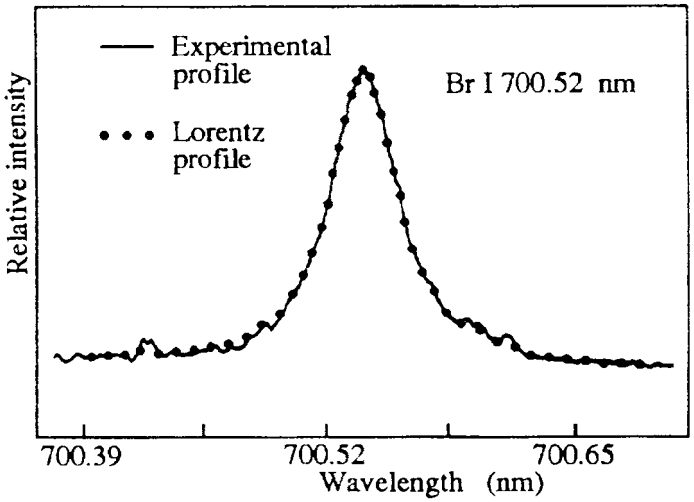

Fig. 5.3 Comparison of experimental and Lorentz profile.

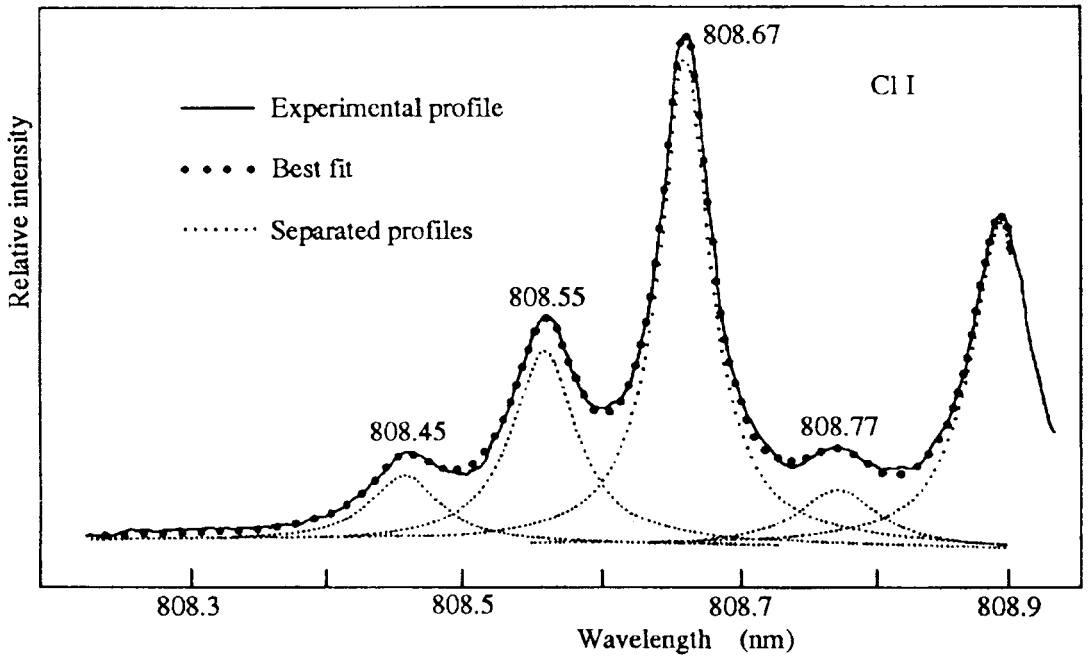

Fig. 5.4 Example of half-width measurements for Cl I $(^1D)\,4s\,^2D - (^1D)\,4p\,^2D^0$ multiplet.

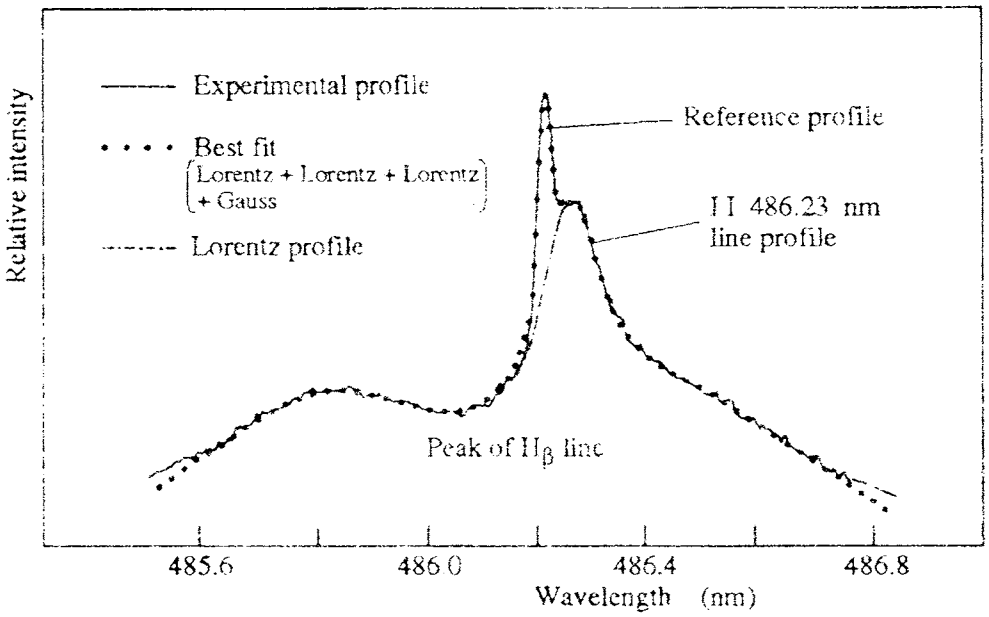

Fig. 5.5 Example of shift measurement for I I 486.23 nm line positioned at the top of the H_β line.

6. EXPERIMENTAL PROFILES OF LINES EMITTED FROM THE PLASMA WITH CYLINDRICAL SYMMETRY

When for some reasons it is necessary to observe the plasma side-on, or, when this is the only way of its observation, the procedure of obtaining experimental profile is more complex than in the case of end-on observations, considered up to now. In this case, the measured radiation intensity contains radiation contributions of a number of layers with the different electron densities and temperatures (Fig. 6.1). If the plasma has a cylindrical symmetry, and if it is optically thin, the experimentally obtained radial profile $I(x)$ recorded along the x axis (see Fig. 6.1) enables evaluation of true radial distribution. In order to separate contributions of particular layers, it is necessary to apply the Abel inversion procedure. The mathematical formulation of the Abel inversion process is as follows. The plasma radiation intensity $I(x)$ is a sum of intensities along the y axis at the distance x (Fig. 6.1), and this can be written as:

$$I(x)\,\Delta x\,\Delta z = \Delta x\,\Delta z \int_{-y}^{y} \varepsilon(r)\; dy \qquad (6.1)$$

where Δx is the observed width, and Δz is the thickness of the plasma layer, determined by the width and height of the monochromator entrance slit, or by the diaphragm, and $\varepsilon(r)$ is the local plasma emissivity, i.e. the emissivity at the distance r from the plasma centre. Because of the symmetry ($I(-x) = I(x)$), equation (6.1) can be written in the form:

$$I(x) = 2 \int_{0}^{y} \varepsilon(r)\; dy \qquad (6.2)$$

The intensity $I(x)$ is also a function of the wavelength, time, etc., but for the sake of simplicity we shall treat it here only as a function of x. In view of the relation $r^2 = x^2 + y^2$, equation (6.2) becomes (Bederson, 1968; Lochte-Holtgreven, 1968):

$$I(x) = 2 \int_{x}^{R} \frac{\varepsilon(r)\, r\, dr}{\sqrt{r^2 - x^2}} \qquad (6.3)$$

This is a form of the Abel integral equation and, if $I(x)$ is equal zero for all $r > R$, equation (6.3) can be inverted into (Hildebrand, 1952; Bracewell, 1986):

$$\varepsilon(r) = -\frac{1}{\pi} \int_{r}^{R} \frac{I'(x)\, dx}{\sqrt{x^2 - r^2}} \qquad (6.4)$$

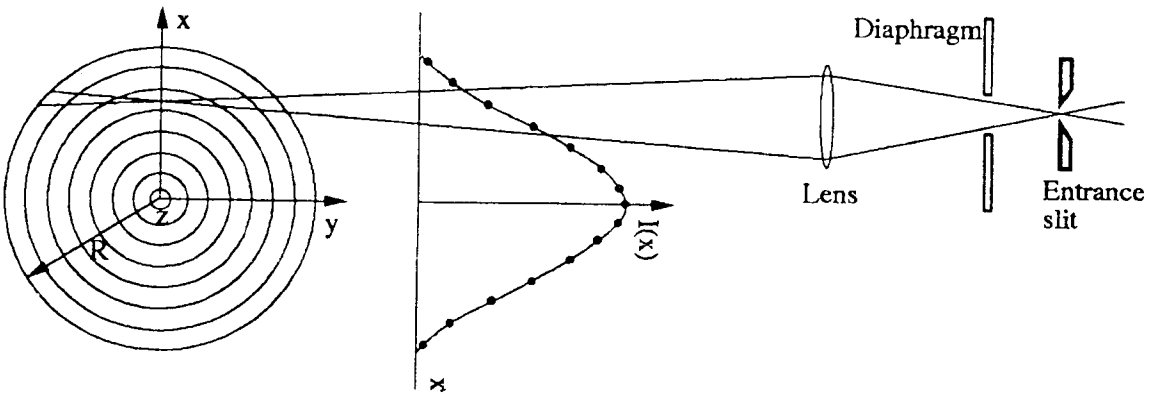

Fig. 6.1 Schematic optical arrangement for radial plasma observations.

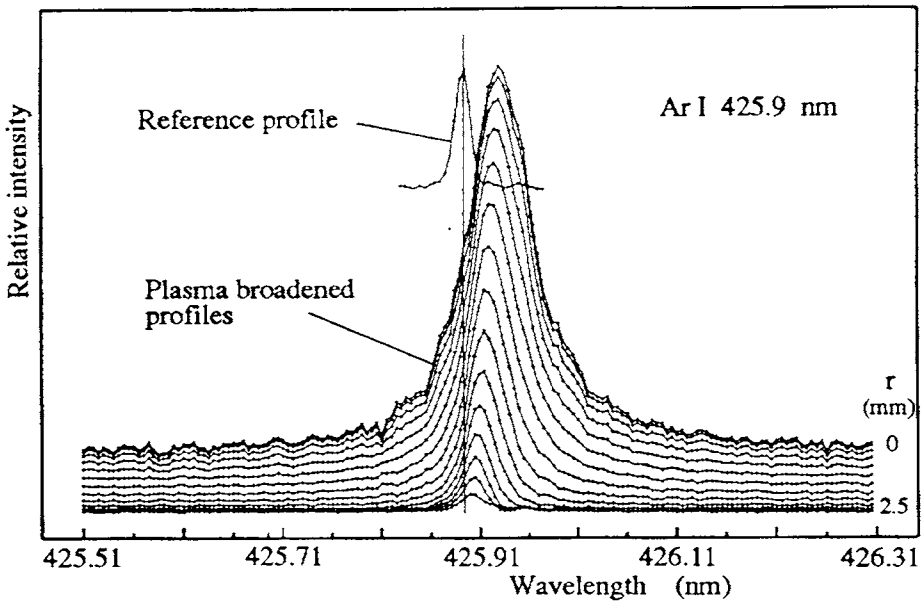

Fig. 6.2 Set of Ar I 425.9 nm line profiles obtained after the Abel inversion procedure.

where $I'(x) = dI(x)/dx$. In practice, $I(x)$ is a set of time-averaged values measured at particular points along the x axis. Because $I(x)$ can not be expressed in an analytical form, equation (6.4) has to be solved numerically, or the experimental distribution is to be approximated by some analytical function. To solve this problem, numerous methods have been developed (Djurović et al., to be published), but this is not the subject of our present concern.

One possible procedure is to record first the radial distribution at each wavelength, in the appropriate steps along the spectral line. Then, for each radial distribution, the Abel inversion (equation 6.4) should be performed. Only after that one can reconstruct profiles of the spectral lines corresponding to the different layers along the plasma radius. An example of the obtained profiles for the Ar I 425.9 nm line emitted from the wall-stabilized electric arc, is presented in Fig. 6.2. The Figure also contains the reference argon line. From these profiles, the experimental half-width and shift can be determined by the procedure that has already been described.

There is also the possibility to apply the Abel inversion onto the plasma sources with a certain asymmetry. Solving of this problem has been described, for example, in Yasutomo et al. (1981).

7. DECONVOLUTION OF EXPERIMENTAL PROFILES

A spectral line emitted from any plasma source is always naturally broadened, and, if recorded by an appropriate spectral apparatus, it has also a certain instrumental width. All other effects influencing spectral line broadening are superimposed onto these two omnipresent effects. In a general case, if two effects cause simultaneous broadening of a spectral line, the resulting profile will not always be an algebraic sum of the profiles due to the individual effects. If one effect can be described by the $A(x)$ function, and the other by the function $B(x)$, then, the resulting spectral distribution is defined by the convolution of these two functions $K(x)$ (Konjević and Roberts, 1976):

$$K(x) = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} A(y)\; B(x-y)\; dy \tag{7.1}$$

If, for example, both functions are of the Gaussian type, the resulting half-width is:

$$\mathrm{w}_{RG} = \left(\mathrm{w}_{G1}^2 + \mathrm{w}_{G2}^2\right)^{1/2} \tag{7.2}$$

This can be used for separation, i.e. deconvolution, of the Doppler and instrumental half-width. If both functions are of the Lorentz type, the resulting half-width is:

$$\mathrm{w}_{RL} = \mathrm{w}_{L1} + \mathrm{w}_{L2} \tag{7.3}$$

However, if the functions $A(x)$ and $B(x)$ are different, deconvolution is more complex. Solution of the problem of separating half-widths in the case of convolution of the Lorentz and Gaussian profile, the so-called Voigt profile, has been described in Davies and Vaughan (1963). The same reference contains the tabulated ratios $k_V^G = \mathrm{w}_G/\mathrm{w}_V$ and $k_V^L = \mathrm{w}_L/\mathrm{w}_V$ as a function of $k_V = \mathrm{w}_{V1/10}/\mathrm{w}_V$, which is graphically presented in Fig. 7.1. Here w_G, w_L, and w_V denote the half-width of the Gaussian, Lorentz and Voigt profile, respectively, and $\mathrm{w}_{V1/10}$ is the width of the Voigt profile at 1/10 of the profile height.

In the deconvolution procedure it is necessary first to determine the coefficient k_V as the ratio $\mathrm{w}_{E1/10}/\mathrm{w}_E$, where w_E is the experimental profile half-width, and $\mathrm{w}_{E1/10}$ is the width of the experimental profile at 1/10 of its height. Then, from Fig. 7.1 the values of coefficients k_V^G and k_V^L, can be read and the sought half-widths of the Gaussian and Lorentz profile can be calculated as:

$$\mathrm{w}_G = k_V^G\; \mathrm{w}_E \tag{7.4}$$

and

$$\mathrm{w}_L = k_V^L\; \mathrm{w}_E \tag{7.5}$$

If the whole procedure is followed correctly, than the values w_G obtained from (7.4) and w_{RG}

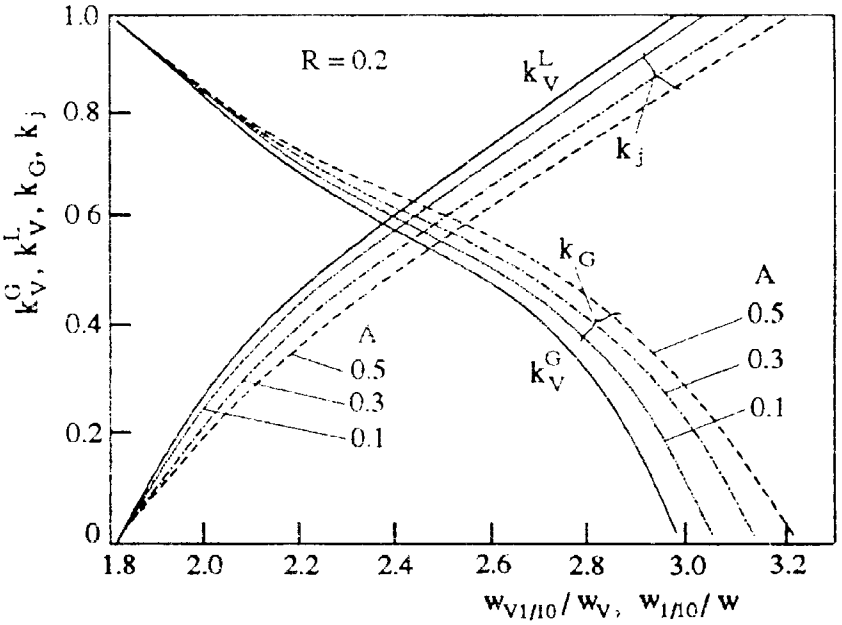

Fig. 7.1 Dependence of coefficients k_V^G and k_V^L on $\mathrm{w}_{V1/10}/\mathrm{w}_V$ ratio and k_G and k_j on $\mathrm{w}_{1/10}/\mathrm{w}$ ratio.

calculated from (7.2), where, for example, w_{G1} ic the Doppler half-width and w_{G2} is the measured instrumental half-width, should be approximately equal.

When the Stark effect is predominant, the obtained value w_L is at the same time the Stark half-width of the line. However, if there is even a small contribution of other effects, for example, van der Waals broadening, a correction has to be carried out with the aid of (7.3).

When the above deconvolution procedure is used for spectral lines of neutral atoms, an error can be made because the Stark profile, which is in fact an asymmetrical $j(x)$ profile, is described by the symmetric Lorentz profile. This is not of great importance when we consider lines for which the ion-broadening parameter has a small value, but for larger A values this error, however, may be significant.

A solution for convolution of $j(x)$ and Gaussian profile

$$K(x) = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} j_{A,R}(y)\; G(x-y)\; dy \qquad (7.6)$$

has been recently given in Mijatović et al. (1993). Because of the complicated analytical form of the $j_{A,R}(x)$ function, the tabulated values (Woltz, 1986), interpolated by a cubic spline, was used. Integration was carried out in the interval -20 to +20 (Woltz, 1986). The error of this approximation is negligible, because at the distance $x = 20$ from the profile centre, the intensity falls practically to zero. The coefficients k_j and k_G are defined in the same way as the corresponding coefficients for the Voigt profile ($k_j = w_j/w$, $k_G = w_G/w$). The values of these coefficients are presented in Fig. 7.1 (dotted lines) as a function of $k = w_{1/10}/w$, for one value of parameter R and three values of parameter A. Deconvolution is also carried out as in the case of the Voigt profile:

$$w_G = k_G\; w_E \qquad (7.7)$$

$$w_j = k_j\; w_E \qquad (7.8)$$

The Debye shielding parameter R can be calculated from (2.4.4), and the ion-broadening parameter A is usually taken from Griem, (1974), or it can be estimated from the approximative formula given in Freudenstein and Cooper, (1978).

If deconvolution of the lines of neutral atoms with the parameter $A = 0.5$ is made using the Voigt profile instead of the convolution of $j(x)$ and Gaussian profile, this may result in an error of up to 25% (Mijatović et al., 1993).

The Stark half-widths extracted from the experimental spectral line profiles can be now used for a comparison with various theoretical values, other experimental data, and for plasma diagnostics.

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ЕКСПЕРИМЕНТАЛНЕ ПОТЕШКОЋЕ КОД ОДРЕЂИВАЊА ОБЛИКА СПЕКТРАЛНИХ ЛИНИЈА ЕМИТОВАНИХ ИЗ ПЛАЗМЕ

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Прегледни чланак

На основу емитованог зрачења и профила спектралних линија могу се добити различите информације о плазми, као сто су на пример, концентрације неутралних и наелектрисаних честица, њихове температуре и подаци о различитим атомским процесима. Овако добијени подаци су од великог значаја како за дијагностику плазме и тестирање теорије тако и за различите примене плазме.

Приликом експерименталног рада, како при снимању профила спектралних линија тако и при њиховој обради настају бројне потешкоће. Овај рад је покушај да се ови проблеми систематизују и да се понуде одговарајућа решења.

У раду је прво дат преглед узрока ширења спектралних линија у плазми као и кратак преглед теорија које описују ширење спектралних линија. Описана је техника снимања профила као и провера и корекција на самоапсорпцију. Такође је разматрана обрада експерименталних профила, тј. одређивање полуширина и помераја спектралних линија. Разматран је и проблем Абелове инверзије која је неопходна у случају извора плазме са цилиндричном симетријом. На крају је детаљно описана процедура издвајања појединих компонената ширења из експерименталног профила линије. Све ово је илустровано бројним експерименталним
примерима.