Mem. S.A.It. Vol. 7, 192
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Memorie della
Supplementi

Measured Stark shifts of Kr I line profiles in the 5s–5p and 5s–5p' transitions

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Abstract. On the basis of the precisely recorded 10 neutral krypton (Kr I) line shapes in the 5s–5p and 5s–5p' transitions, it has been obtained the Stark shift. These lines have been studied in a linear, low–pressure, optically thin pulsed arc discharge operated in pure krypton. The line shapes are measured at 17 000 K electron temperature (T) and at 16.5x10^{22} m^{-3} electron density (N). The mentioned plasma parameters have been measured using independent experimental diagnostics techniques, as well as from the line deconvolution procedure. The separate electron and ion contributions from the total Stark shift (d_{t}), i.e. d_{e} and d_{i} have been obtained and represent the first experimental data in this field. On the basis of the observed asymmetry of the Stark broadened line profile it was deduced the ion broadening parameters which describe the influence of the ion static and the ion–dynamical effect on the shift of these 10 Kr I line shapes.

Key words. Line shapes, widths, and shifts; Neutrals in plasmas; Plasma diagnostic techniques and instrumentation

1. Introduction

Stark broadening in plasmas is important to theoretical understanding as well as for experimental methods, e.g. as a diagnostic tool. Plasma broadened and shifted spectral line profiles have been used for a number of years as a basis of an important non–interfering plasma diagnostic technique. Numerous theoretical and experimental efforts have been made to find solid and reliable basis for this application. This technique became, in some cases, the most sensitive and often the only possible plasma diagnostic tool (Griem 1964).

In this paper is presents the measured Stark shift of the ten Kr I spectral line (in 5s–5p and 5s–5p' transitions) at about 17 000 K electron temperature and at about 16.5x10^{22} m^{-3} electron density. The values of T, used in our analysis, are typical for many cosmic light sources and laboratory plasmas. On the basis of the observed Kr I line profile asymmetry, the characteristics of the ion contribution to the total Stark shift (d_{t}), as expressed by the ion–static parameter (A) and the ion–dynamical parameter (E) are obtained. As an optically thin plasma source we are used a linear, low–pressure, pulsed arc operated in pure krypton discharge.

Up to now only three experimental works (Klein & Meiners 1977; Vitel & Skowronek 1987; Uzelac & Konjević 1989) are devoted to the Kr I Stark sift investigation of spectral lines from 5s–5p' transition. In these experiments the symmetrical Voigt or Lorentz line profiles were used for deconvolution procedure giving Stark shift values generated by electrons without estimation the ion component (d_i) generated by Kr II ions (or other ions) (Lesage & Fuhr 1999; Konjević 2002; NIST 2005) in the total Stark shift (d_t).

It this paper the d_t, d_e and d_i values are compared to available experimental Stark broadening parameters and indirectly with the semiclassical perturbation formalism (SCPF) (Dimitrijević 2005).

2. Theoretical background and deconvolution procedure

The total line Stark shift (d_t) with the corresponding electron d_e and ion d_i contributions is given by:

$$d_\mathrm{t} = d_\mathrm{e} + d_\mathrm{i} \tag{1}$$

In this way it makes the difference between $d_\mathrm{t,\ st}$ and $d_\mathrm{t,\ s+d}$. The $d_\mathrm{t,\ st}$ is total "static" Stark shift. The "static" means semiclassical theory by the Griem's theory (Griem 1964, 1974). The $d_\mathrm{t,\ s+d}$ is total "static and dynamic" Stark shift. The "static and dynamic" has same meaning as introduced by Kelleher (1981).

So, for a non–hydrogenic, isolated neutral atom line the ion broadening is not negligible and the line profiles are described by an asymmetric K function (see Eq. (6)). The $d_\mathrm{t,\ st}$ and $d_\mathrm{t,\ s+d}$ may be calculated from the equations (Griem 1974; Kelleher 1981):

$$d_\mathrm{t,\ st} \approx W_\mathrm{e}[d_\mathrm{e}/W_\mathrm{e} \pm 2A(1-0.75R)]$$

and

$$d_\mathrm{t,\ s+d} \approx W_\mathrm{e}[d_\mathrm{e}/W_\mathrm{e} \pm 2AE(1-0.75R)] \tag{2}$$

where

$$R = \sqrt[6]{\frac{36 \cdot \pi \cdot e^6 \cdot N}{(kT)^3}}, \tag{3}$$

is the so called Debye shielding parameter, i.e. the ratio of the mean ion separation to the Debye radius, where k is the Boltzmann constant, the W_e is corresponding Stark electron FWHM, N and T represent the electron density and temperature respectively. A is the quasi–static ion broadening parameter (see Eq. (224) in Griem (1974)), E is a coefficient of the ion–dynamical contribution to the shift, with the established criterion (Kelleher 1981):

$$E = \frac{2.35 \cdot B^{-1/3} - 3A^{1/3} \cdot R}{2 \cdot (1 - 0.75 \cdot R)} \qquad \text{for} \qquad B < 1;$$

or

$$E = 1 \qquad \text{for} \qquad B \geq 1, \tag{4}$$

where

$$B = A^{1/3} \cdot \frac{4.03 \cdot 10^{-7} \cdot W_e[\mathrm{nm}]}{(\lambda[\mathrm{nm}])^2} \cdot (N[\mathrm{m}^{-3}])^{2/3} \cdot$$

$$\sqrt{\frac{\mu}{T_\mathrm{g}[\mathrm{K}]}} < 1; \tag{5}$$

is the factor with atom–ion perturber reduced mass μ (in amu) and gas temperature T_g (Kelleher 1981). When $E = 1$ the influence of the ion–dynamic effect on the shift is negligible and the line shape is treated using the quasi–static ion approximation, i.e. $d_\mathrm{t,\ s+d}$=$d_\mathrm{t,\ st}$, described by Milosavljević & Poparić (2001) and references therein:

$$K(\lambda) = K_\mathrm{o} + K_\mathrm{max} \int_{-\infty}^{\infty} exp(-t^2) \cdot$$

$$\left[\int_0^{\infty} \frac{\mathrm{H_R}(\beta)}{1 + (2\frac{\lambda - \lambda_\mathrm{o} - \frac{\mathrm{W_G}}{2\sqrt{ln2}} \cdot \mathrm{t}}{\mathrm{W_e}} - \alpha \cdot \beta^2)^2} \cdot d\beta\right] \cdot dt. \tag{6}$$

Here K_o is the baseline (offset) and K_max is the maximum intensity (for λ=λ_o) (Milosavljević & Poparić 2001). $H_\mathrm{R}(\beta)$ is the electric microfield strength distribution function of normalized field strength β=F/F_o, where F_o is the Holtsmark field strength. A (α=$A^{4/3}$) is the quasi–static ion broadening parameter and represents the measure of the relative importance of ion and electron broadenings. R is the Debye shielding parameter (see Eq. (3)) and W_e is the electron width (FWHM) in the $j_{A,R}$ (Milosavljević & Poparić 2001; Griem 1974) plasma broadened spectral line profile. The Gaussian FWHM width W_G is given by Eq. (7) (i.e the Eq.(2.3) in Milosavljević & Poparić (2001)).

$$W_G = 2 \cdot \sqrt{\frac{2 \cdot \ln 2 \cdot kT}{m}} \cdot \frac{\lambda_o}{c}. \tag{7}$$

Here, T is the emitter equivalent kinetic temperature, m is its mass, and k and c are the Boltzmann constant and velocity of the light, respectively.

The fitting procedure with the K–convolution integral is tested using another set of experimental data (see Milosavljević & Djeniže (2002a,b,c, 2003a,b,c); Milosavljević et al. (2003a,b, 2004a,b); Milosavljević & Poparić (2003)), as well. The K convolution integral is used for the analysis of our new data for many spectral lines of neutral rare gases. By comparing the different spectral lines obtained under the same plasma conditions, we tested the physical stability of the deconvolution procedure. All details about deconvolution and fitting procedure is described in earlier publications (Milosavljević & Poparić 2001, 2003; Milosavljević et al. 2003a; Milosavljević 2001).

3. Experiment

The modified version of the linear low–pressure pulsed arc (Djeniže et al. 1991, 1998, 2002; Milosavljević et al. 2000, 2001) has been used as a plasma source. A pulsed discharge was performed in a quartz discharge tube of 5 mm inner diameter and plasma length of 7.2 cm. The tube has end-on quartz window. On the opposite side of the electrodes the glass tube was expanded in order to reduce erosion of the glass wall and also sputtering of the electrode material onto the quartz windows. The working gas was pure krypton (99.9999%) at 133 Pa filling pressure in flowing regime. Spectroscopic observation of isolated spectral lines has been made end-on along the axis of the discharge tube. A capacitor of 14 μF was charged up to 1.5 kV. The line profiles were recorded using a shot-by-shot technique with a photomultiplier (EMI 9789 QB and EMI 9659B) and a grating spectrograph (Zeiss PGS-2, reciprocal linear dispersion 0.73 nm/mm in first order) system. The instrumental FWHM of 8 pm was determined by using the narrow spectral lines emitted by the hollow cathode discharge. The recorded profiles of these lines are Gaussian in shape within 8% accuracy within the range of the investigated spectral line wavelengths. The spectrograph exit slit (10 μm) with the calibrated photomultiplier was micrometrically traversed along the spectral plane in small wavelength steps (7.3 pm). The averaged photomultiplier signal (five shots at the same spectral range) was digitized using an oscilloscope, interfaced to a computer. A sample output are shown in Figure 1 in Milosavljević et al. (2003a).

Plasma reproducibility is monitored by the Kr I and Kr II line radiation and, also, by the discharge current using a Rogowski coil signal (it was found to be within ±5%).

To check existence of the self–absorption, relative line intensity (I) ratio is controlled during the plasma decay (Djeniže & Bukvić 2001), as well as by doubling optical path length (Konjević 1999; Milosavljević 2001). No evidence for the self–absorption is found for these ten Kr I spectral lines. Namely in the case of these atomic krypton lines are found the constant relative line intensity ratio (Djeniže & Bukvić 2001). As it works with pulsed plasma source, the constant mean constant first 150–200 μs after beginning of discharge.

The plasma parameters (N and T) were determined independently using standard diagnostics methods. Diagnostical methods and used procedures have been described, in detail, in the work Milosavljević et al. (2000). Thus, electron temperature (T^{exp}) decay is obtained by using the Saha equation applied for Kr II and Kr I line intensity ratios. Electron density (N^{exp}) decay is obtained using laser interferometry technique. Temporal evolution of T^{exp} and N^{exp} are presented in Figure 2 in Milosavljević et al. (2003a).

4. Results and Discussion

The experimentally obtained $d_t^{\rm exp}$, $d_e^{\rm exp}$, $d_i^{\rm exp}$ and $E^{\rm exp}$ data, together with those of other authors are presented in Table 1. $d_{\rm t,\,s+d}^{\rm exp}$ and $d_{\rm t,\,st}^{\rm exp}$ mean total Stark shift with included static+dynamic and static only ions contribution, respectively (see Eq. 2). The data for $A^{\rm exp}$ and W_e are published previously in the papers Milosavljević & Djeniže (2002c); Milosavljević et al. (2003a).

In the Table 1, beside the data presented in this paper, there is the three more experiments dealing with Stark shift. In these three experimental works, only measurements for two lines from the Table 1 are present.

This most investigated line in the Table 1 is the line 587.092 from 5s–5p' transition. This line are also investigatived by Klein & Meiners (1977); Vitel & Skowronek (1987); Uzelac & Konjević (1989) and in absences of any theoretical calculation it is difficult to make any comparatione. In the Vitel & Skowronek (1987) is present one plasma condition which is close by electron temperature to the electron temperature of results presented in this paper. In this analysis could be found that the Stark sift of the line 587.092 nm line in Vitel & Skowronek (1987) is about 25% less than present in this paper. This discrepancy could be explained by using the wrong convoluting integral in the paper of Vitel & Skowronek (1987) i.e. using the symmetrical Voigt/Lorentz line profiles instead of asymmetric $j_{R,A}$/K function (Griem 1974; Milosavljević 2001) .

The theoretical calculation (SCPF) (Dimitrijević 2005) has been done only for Kr I lines from 5s–5p transition. The accuracy of energy for perturbation levels was the problem to perform similar calculation (Dimitrijević 2005) for the Kr I lines from 5s–5p' transition.

In the Figs. 1 and 2 are present the ratio of data from this paper and from SCPF calculation (Dimitrijević 2005).

Taking in account the uncertainties of the shift (±12%), electron density (±7%) and temperature (±9%) measurements, the agreement between the calculated and measured data is very well.

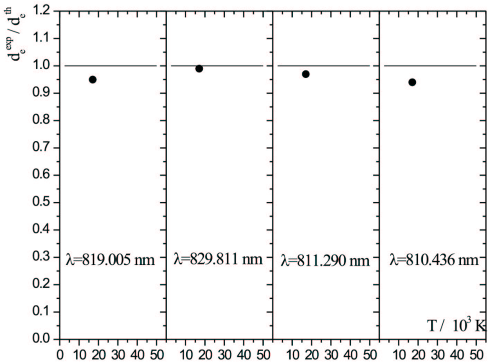

Fig. 1. Ratios of the experimental $d_e^{\rm exp}$ and the calculated $d_e^{\rm th}$ (Dimitrijević 2005) electron Stark widths vs. electron temperature for the most investigated Kr I spectral lines belonging to the 5s-5p transition. •, the experimental results presented in this paper.

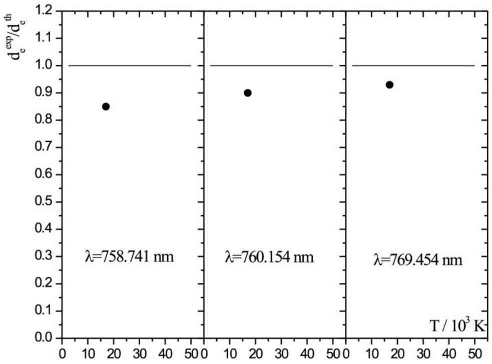

Fig. 2. Same as figure 1, but for other three lines from 5s–5p transition.

5. Conclusions

It is shown that the line deconvolution procedure, applied to 10 Kr I line profiles, gives convenient plasma parameters (N and T) at about 17 000 K electron temperature and 1.6x10^{23} m^{-3} electron density, and recommending this method for plasma diagnostics purposes for the case of optically thin plasmas.

It has been found that the electron contribution ($d_e^{\rm exp}$) is about 88%, and the Krypton ions

Table 1. The Kr I line broadening characteristics. Measured: $d_{\mathrm{t}}^{\mathrm{exp}}$, $d_{\mathrm{e}}^{\mathrm{exp}}$ and $d_{\mathrm{i}}^{\mathrm{exp}}$ within 12% accuracy at measured electron temperature (T^{exp}) and electron density (N^{exp}). Ref represents experimental values given in this work (Tw) and those used from other authors: KM, Klein & Meiners (1977); VS, Vitel & Skowronek (1987); UK, Uzelac & Konjević (1989). Also, with (exp) are denoted experimental data; (t) – total; (i) – ion; (e) – electron; (st) – static only; (s+d) – static and dynamic.

Transition	Multiplet	λ [nm]	T^{exp} [10^3K]	N^{exp} [$10^{22}\mathrm{m}^{-3}$]	$d_{\mathrm{t,\,s+d}}^{\mathrm{exp}}$ [pm]	$d_{\mathrm{t,\,st}}^{\mathrm{exp}}$ [pm]	$d_{\mathrm{e}}^{\mathrm{exp}}$ [pm]	$d_{\mathrm{i}}^{\mathrm{exp}}$ [pm]	E^{exp}	Ref.
5s–5p	$[3/2]^{o}_{1}$-$[1/2]_{o}$	758.741	17.0	16.5	136.8	131.6	124.1	12.7	1.69	Tw
	$[3/2]^{o}_{2}$-$[3/2]_{2}$	760.154	17.0	16.5	101.1	96.0	89.5	11.6	1.80	Tw
	$[3/2]^{o}_{2}$-$[3/2]_{1}$	769.454	17.0	16.5	98.3	93.3	88.2	10.1	1.98	Tw
	$[3/2]^{o}_{1}$-$[3/2]_{2}$	819.005	17.0	16.5	117.1	111.1	104.2	12.9	1.85	Tw
	$[3/2]^{o}_{1}$-$[3/2]_{1}$	829.811	17.0	16.5	116.2	110.3	103.8	12.4	1.92	Tw
	$[3/2]^{o}_{2}$-$[5/2]_{3}$	811.290	17.0	16.5	94.8	89.0	82.1	12.7	1.84	Tw
	$[3/2]^{o}_{2}$-$[5/2]_{2}$	810.436	17.0	16.5	93.8	87.9	79.9	13.9	1.74	Tw
5s–5p’	$[3/2]^{o}_{2}$-$[1/2]_{1}$	557.029	17.0	16.5	55.0	55.0	48.7	6.3	1.00	Tw
			10.3 – 9.4	10	21.5					KM
	$[3/2]^{o}_{2}$-$[3/2]_{2}$	556.222	17.0	16.5	52.7	50.2	44.7	8.0	1.46	Tw
	$[3/2]^{o}_{1}$-$[3/2]_{2}$	587.092	17.0	16.5	51.0	48.1	42.4	8.6	1.51	Tw
			10.3 – 9.3	10	21.8					KM
			15.5	76	190					VS
			14.9	92	200					VS
			14.3	97	210					VS
			16.2	123	250					VS
			15.0	124	250					VS
			17.4	158	300					VS
			15.7	162	320					VS
			11.5	45	100					UK
			11.65	64	130					UK
			11.9	76	160					UK
			12.5	87	190					UK
			12.75	102	190					UK

(Kr II, Kr III, ...) contribution is about 12% (on average), to the total Stark shift.

Very good agreement was found among all existing $\mathrm{d}_{\mathrm{e}}^{\mathrm{exp}}$ and the $\mathrm{d}_{\mathrm{e}}^{\mathrm{SCPF}}$ values for the 7 Kr I spectral lines from 5s-5p transition.

It has found a clear influence of the quasi-static ion and ion dynamic effects on the investigated spectral line shapes. They play an important role, especially for the Kr I spectral lines from 5s–5p transition.

The observed ion dynamic effect, at our plasma conditions, increase the quasi-static ion contribution for about 5% . This might play an important role for the use of these lines for astrophysical plasma modeling or for diagnostics purposes.

Acknowledgements. This work is a part of the project OI1228 ”Determination of the atomic parameters on the basis of the spectral line profiles” supported by the Ministry of Science and Environment Protection of the Republic of Serbia. The author is grateful to Science Foundations Ireland under grand No.: 02/IN.1/I147 and European Union founding under EURATOM contract FU06-CT-2004-00068, fo their support.

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