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Stark broadening of Si II and Si III spectral lines

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Summary. Modified semiempirical and approximative semi-classical methods have been used for the calculation of recently measured Si II and Si III Stark line widths in order to test both methods, as well as the new experimental data (Kusch and Schröder, 1982).

Key words: plasma spectroscopy – silicon – line broadening

Introduction

Stark broadening parameters for silicon spectral lines are useful for a number of astrophysical problems. Reliable data are required for the evaluation of the physical conditions in the stellar plasma as well as for the opacity calculations, since the silicon takes the sixth place in the stellar abundance of elements (Unsöld, 1967). In spectra of hot stars of B and A type the Si II spectral lines are usually present. During the spectral investigation of some peculiar stars of types mentioned, especially the silicon Ap-stars, a large number of less intensive Si II and Si III lines is observed (Jaschek and Garcia, 1966; Hohlova and Ryabtchikova, 1970). Also, silicon lines are often among the principal impurity lines in the analysis of the plasma radiation during laboratory and nuclear fusion research.

For calculation of Stark broadening parameters one can use various more or less sophisticated theoretical approaches (see e.g. Griem, 1974). In particular cases e.g. when a large number of theoretical data are required, or there is not enough data for a reasonable set of perturbing energy levels, or when with the sophistication of calculations the relevant increase of accuracy is not satisfactory due to the complexity of investigated spectrum, simple approximative formulae with good average accuracy may be very useful.

The simple semi-empirical method (Griem, 1968) agrees in average within 50% with the experimental data for singly ionized atoms (Griem, 1974). For multiple ionized atoms the agreement becomes worse and few attempts have been made to extend the applicability of this approach to higher ionization stages (Hey, 1977; Dimitrijević and Konjević, 1980; 1981a; 1981b; Hey and Breger, 1980). For the modified semi-empirical formula (Dimitrijević and Konjević, 1980; 1981a) the average ratio of measured to calculated widths is 1.06 ± 0.31 for doubly- and 0.91 ± 0.42 for triple-charged ions (Dimitrijević and Konjević, 1980). It is interesting that the worse agreement between numerical and experimental values is just for Si III lines (the average ratio of measured to calculated line widths is only 0.67 for this case).

New experimental results for Stark broadening parameters for prominent Si II and Si III lines, have been published recently (Kusch and Schröder, 1982). A number of references concerning experimental and numerical determination of Si II and Si III Stark broadening parameters (Sahal-Bréchot, 1969; Yukov, 1972; Lesage et al. 1977; Hey, 1977c; Platiša et al., 1977; Dimitrijević and Konjević, 1980; 1981a) have not been taken into account in that paper and it is interesting to compare these new experimental data with previously published results. Also, the modified semi-empirical, and approximative semi-classical calculations of Stark widths for Si II and Si III lines have been performed in order to test both methods in the case of Si II and Si III lines, as well as the new experimental data.

Theory

Within the impact approximation Baranger (1958) has derived the quantum-mechanical expression for the width of an isolated ion line:

$$W = N\left\{v\left[\sum_{i'}\sigma_{i'i} + \sum_{f'}\sigma_{f'f}\right]\right\}_{av} + W_{el} \tag{1}$$

where W is the full half-width (FWHM) in units of angular frequency and N is the electron concentration. The symbols $\sigma_{i'i}$ and $\sigma_{f'f}$ represent the inelastic cross sections for collisional transitions to i', f' from initial (i) and final (f) levels, respectively, of the optically allowed transition. W_{el} is the line width induced by elastic collisions. The averaging in Eq. (1) has to be performed over the electron velocity (v) distribution.

Griem (1968) assumed that the contribution of elastic collisions to the line width can be neglected for higher electron temperatures. The same author made an attempt to take elastic collisions into account at the low temperature limit by using the threshold value of the inelastic cross section below the threshold. Within the framework of the dipole approximation, using Bethe's (1930) relation for cross sections together with semi-empirical effective Gaunt-factor approximation proposed by Seaton (1962) and Van Regemorter (1962), we can calculate Stark line width from the well known semi-empirical formula (Griem, 1968)

$$W = N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}} \cdot\left[\sum_{i'}\boldsymbol{R}^2_{j'j}\,g\left(\frac{E}{\Delta E_{i'i}}\right) + \sum_{f'}\boldsymbol{R}^2_{f'f}\,g\left(\frac{E}{\Delta E_{f'f}}\right)\right]. \tag{2}$$

In this expression $R^2_{j'j}$ (in units of the Bohr radius a_0^2) is the square of the coordinate operator matrix element summed over all components of the operator and the magnetic substates of total angular momentum J', and averaged over the magnetic substates of J; $E=3kT/2$ is the energy of the perturbing electron and $\Delta E_{j'j}=|E_{j'}-E_j|$ is the energy difference between levels j and j'. The semi-empirical effective Gaunt factor $g(x)=0.20$ for $x\leqq 2$ and $g(x)=0.24$, 0.33, 0.56, 0.98 and 1.33 for $x=3$, 5, 10, 30, and 100.

For singly ionized atoms semi-empirical formula agrees in average within 50% with the experiment (Griem, 1974). Griem (1974) suggested that this formula can be used for multiple ionized atoms as well, but with an uncertainty of $\pm 100\%$. However, the comparison with the experimental data for doubly- and triply-ionized atoms (Hey, 1976; 1977a; 1977b; Hey and Bryan, 1977; Bogen, 1972; Platiša et al., 1977; 1979) shows that the calculated values are systematically lower. This is an indication that the threshold value $g=0.2$ is rather small for multiple ionized atoms. For multiple ionized atoms it is also sometimes difficult to complete a reasonable set of atomic energy levels since data for higher perturbing levels are often missing in the literature.

To overcome these difficulties and further improve semi-empirical method one can separate transitions to the perturbing levels in three groups (Dimitrijević, and Konjević, 1980; 1981a): transitions with (i) $\Delta n=0$, $l\to l+1$; (ii) $\Delta n=0$, $l\to l-1$, (iii) $\Delta n\neq 0$ (as was used previously by Kobzev (1971) and Griem (1974) within the semi-classical method). Within each group of transitions, matrix elements are treated lumped together. For the transitions with the principal quantum number n unchanged, Bely (1966) found that near threshold values of g could be significantly larger than 0.2. A study of transitions of this type has been made by Blaha (1969) for 15 different isoelectronic sequences. He finds threshold values of g ranging from 0.31 to 0.96. Kobzev (1971) suggested an empirical value of $g=0.9-1.1/z$ at threshold, which is in agreement with the conclusion of Blaha (1969). We have adopted this suggestion calculating the Gaunt factor for higher electron energies from the following equation:

$$\tilde{g}(x)=0.7-1.1/z+g(x) \tag{3}$$

For transitions with $\Delta n\neq 0$, $g=0.2$ at threshold is retained and the energy separation to the nearest perturbing level is estimated from

$$\Delta E_{n,n+1}\approx 2Z^2E_H/n^{*3}, \tag{4}$$

where Z is the charge "seen" by the optical electron ($Z=1$ for neutrals, 2 for singly charged ions etc.) and n^* is the effective principal quantum number.

Equation (1) becomes now

$$\begin{aligned}W=N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\Bigg[&\boldsymbol{R}^2_{l_i,l_i+1}\tilde{g}\left(\frac{E}{\Delta E_{l_i,l_i+1}}\right)+\boldsymbol{R}^2_{l_i,l_i-1}\tilde{g}\left(\frac{E}{\Delta E_{l_i,l_i-1}}\right)\\&+\boldsymbol{R}^2_{l_f,l_f+1}\tilde{g}\left(\frac{E}{\Delta E_{l_f,l_f+1}}\right)+\boldsymbol{R}^2_{l_f,l_f-1}\tilde{g}\left(\frac{E}{\Delta E_{l_f,l_f-1}}\right)\\&+\sum_{i'}(\boldsymbol{R}^2_{ii'})_{\Delta n\neq 0}g\left(\frac{3kTn_i^{*3}}{4Z^2E_H}\right)+\sum_{f'}(\boldsymbol{R}^2_{ff'})_{\Delta n\neq 0}g\left(\frac{3kTn_f^{*3}}{4Z^2E_H}\right)\Bigg].\end{aligned} \tag{5}$$

Relevant matrix elements can be calculated using Coulomb approximation of Bates and Damgaard (1949)

$$\boldsymbol{R}^2_{l,l'}\simeq\left(\frac{3n^*}{2Z}\right)^2\frac{\max(l,l')}{2l+1}[n^{*2}-\max^2(l,l')]\phi^2 \tag{6}$$

$$\sum_{j'}(\boldsymbol{R}^2_{jj'})_{\Delta n\neq 0}\simeq\left(\frac{3n_j^*}{2Z}\right)^2\frac{1}{9}(n_j^{*2}+3l_j^2+3l_j+11),\quad j=i,f. \tag{7}$$

Here, ϕ represents the Bates-Damgaard factor [tabulated e.g. in Oertel and Shomo's (1968) paper].

At higher electron temperatures (Say $3kT/2\Delta E>50$), all Gaunt factors are calculated in accordance to the GBKO (Griem et al., 1962) high temperature limit, viz.

$$\tilde{g}_{j'j}=g_{j'j}=\frac{\sqrt{3}}{\pi}\left[\frac{1}{2}+\ln\left(\frac{2ZkT}{n_j^{*2}\Delta E_{j'j}}\right)\right]. \tag{8}$$

Modified semi-empirical formula, Eq. (5), is very similar in form to the equation for isolated line widths of multiple-charged ions derived by Griem (1974) within the semi-classical-perturbation formalism and slightly modified recently (Dimitrijević and Konjević, 1980), i.e.

$$\begin{aligned}W=N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\int_0^\infty\frac{f(v)}{v}dv\Bigg\{&\Bigg[\left(\boldsymbol{R}^2\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{l_i,l_i+1}+\left(\boldsymbol{R}^2\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{l_i,l_i-1}\\&+\left(\boldsymbol{R}^2\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{l_f,l_f+1}+\left(\boldsymbol{R}^2\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{l_f,l_f-1}\Bigg]_{\Delta n=0}\\&+\sum_{i'}(\boldsymbol{R}^2_{i'i})_{\Delta n=0}\left(\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{n_i,n_i+1}\\&+\sum_{f'}(\boldsymbol{R}^2_{f'f})_{\Delta n=0}\left(\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{n_f,n_f+1}\Bigg\}+\mathrm{W}_{c'},\end{aligned} \tag{9}$$

$$\left(\ln\frac{\varepsilon_{\max}}{\varepsilon_{\min}}\right)_{l,l'}=\ln\left\{1.4+\xi_{l,l'}^{-1}\left[1+\frac{mv^2n_l^{*2}}{2E_HZ(Z-1)}\right]^{-1}\right\},$$

$$\xi_{l,l'}=\frac{(Z-1)e^2\omega_c}{mv^3}, \tag{10}$$

$$\omega_c=\max\{|\omega_{l,l'}|,\omega_P,\omega_F,\Delta\omega_i\}.$$

Here, ε is the eccentricity of the hyperbolic perturber path, $\omega_{l,l'}$ is the frequency separation between, l,l' levels, $\omega_P=(4\pi Ne^2/m)^{1/2}$ is the plasma frequency, ω_F is the fine structure splitting, and $\Delta\omega_i$ is the ion splitting. Furthermore, since the $n\to n+1$ transitions dominate between all $n\neq 0$ contributions, one should take $\hbar\omega_c\approx 2Z^2E_H/n^{*-3}$.

In Eq. (9), W_c is the line width induced by strong collisions and higher multipole interactions, i.e.

$$W_c=2\pi N\left(\frac{2m}{\pi kT}\right)^{1/2}\left(\frac{\hbar}{mZ}\right)^2n_i^{*4}\left[1+\frac{kT}{E_H\left(1+\frac{kT}{E_H}+\frac{Z^2}{n_i^{*4}}\right)}\right]. \tag{11}$$

Comparisons with reliable experimental data for doubly-ionized atoms yield, as an average ratio of measured to calculated widths, 1.06 ± 0.31 for the modified semi-empirical and 0.96 ± 0.24 for the approximative semi-classical method (Dimitrijević and Konjević, 1980). For triply ionized atoms these ratios are 0.91 ± 0.42 and 1.08 ± 0.41 respectively.

Results and discussion

All atomic data needed for calculations were taken from Moore (1965). The Key data on all experiments discussed in this paper are systematized in Table 1. The results of various experimental

Table 1. Key data on experiments

Ref.	Plasma source	Method of measurement		
		Electron density	Temperature	Spectrum
Miller (1968) Lesage and Miller (1975) Lesage et al. (1977)	Gas driven shock tube	H_β Stark width	Line reversal technique applied to H_α line, absolute intensity of NeI 5852 Å line and H_β	Photographicaly
Purić et al. (1974)	T-tube	Laser interferometry at 6328 Å	Boltzmann plot of ArII line intensities	Photoelectricaly, shot by shot
Platiša et al. 1977	Low pressure pulsed arc	Laser interferometry at 6328 Å	Boltzmann plot of ClIII line intensities	Photoelectricaly, shot by shot
Kusch and Schröder 1982.	Pulsed discharge	H_β Stark width	Ratio of the SiIII - line 3791 Å and the SiII-line 5979 Å	Photographicaly

Table 2. Experimental and theoretical Stark widths (FWHM) of Si II. Experimental data: W_M: Miller (1968); W_{LM}: Lesage and Miller (1975); W_{LSM}: Lesage et al. (1977); W_{KS}: Kusch and Schröder (1982). Theoretical data: W_{JBG}: Jones et al. (1971); W_{ASC}: Present approximative semiclassical calculations; W_{SB}: Sahal-Bréchot (1969); W_{CO}: Calculations of Bengston according to Cooper and Oertel (1967, 1969) given in Lesage et al. (1977); W_Y: Yukov (1972); W_{SEM}: Present calculations according to modified semi-empirical approach; W_{SE}: semi-empirical calculations (Hey, 1977c)

Ion	Transition multiplet	Wavelength	T(K)	Experimental data (Å)				Theoretical data (Å)						
				W_M	W_{LM}	W_{LSM}	W_{KS}	W_{JBG}	W_{ASC}	W_{SB}	W_{CO}	W_Y	W_{SEM}	W_{SE}
SiII	$4p^2P^o$-$4d^2D$ (5)	5041.03	10000	3.0	3.5	2.53		2.90	2.94	2.62	2.2	2.0	1.76	1.96
			23500				3.90	2.66	2.34				1.41	
		5056.31	10000	3.0	3.5	2.69		2.90	2.94	2.62	2.2	2.0	1.76	1.96
			23500				4.53	2.66	2.34				1.41	
SiII	$4p^2P^o$-$5s^2S$ (4)	5957.56	10000	2.4	3.3	2.78		2.58	3.86	2.83	2.5		2.60	2.55
			23500				3.69	2.30	3.14				2.02	
		5978.93	10000	2.4	3.3	2.75		2.58	3.86	2.83	2.5		2.60	2.55
			23500				4.08	2.30	3.14				2.02	
SiII	$4p^2P^o$-$6s^2S$ (6)	3339.82	23500				0.273	1.90	2.77				2.16	
		3333.14	23500				0.249	1.90	2.77				2.16	
SiII	$3d'^2D^o$-$4p'^2P$ (7.26)	4190.72	23500				0.435		0.528				0.280	
		4198.13	23500				0.446		0.528				0.280	
SiII	$3d'^4F^o$-$4p'^4D$ (7.33)	5688.81	23500				0.835		0.906				0.480	
		5701.37	23500				0.789		0.906				0.480	
		5706.37	23500				0.725		0.906				0.480	

and numerical data for Si II Stark line widths are compared in Table 1 with experimental data of Kusch and Schröder (1982). Experimental full Stark widths (FWHM) of Lesage et al., (1977) (W_{LSM}) are the final result of a series of measurements [Miller, 1968 (W_M); Lesage and Miller (1975) (W_{LM})] and they are systematically lower than the values of Kusch and Schröder (1982) (W_{KS}). The semiclassical half-halfwidths (HWHM) of Jones et al. (1971) (W_{JBG}) [given also in Griem's (1974) book] are erroneously interpreted as full-halfwidths (FWHM) in the paper of Kusch and Schröder (1982). We can see that particularly large difference (a factor of 7) between experimental semiclassical values exists for the multiplet 6, indicating possibly a typing error in the order of magnitude.

Present approximative semiclassical calculations according to Eq. 9 (W_{ASC}) and modified semiempirical calculations according to Eq. 5 (W_{SEM}) are compared in Table 2 with various semiclassical

calculations and experimental results. If we compare present approximative calculations with experimental results of Lesage et al. (1977) and with other, more sophisticated semiclassical calculations, we can conclude, taking into account the simplicity of the approach, that both methods can be used for the estimate of the Stark widths in the case of transitions between configurations with the core ^1S (multiplets 4, 5, 6). In the case of transitions between configurations with the core ^3P (multiplets 7.26 and 7.33), we can see that a difference of the factor of 2 exists between approximate semiclassical and modified semi-empirical results, indicating that the semi-empirical Gaunt factors are too small in this case. One can notice that in all previously investigated cases (Dimitrijević and Konjević, 1980; 1981a; 1981b) the agreement of modified semi-empirical approach with reliable data was better. One must take into account that in present case perturbing energy level structure is complex. This is particularly case for 7.26 and 7.33 multiplets where the $3d'$ levels are the closest perturbing levels for the $4p'$ energy levels and where for $n=3$ only $3d'$ levels exist. If we analyse, as an example, the contribution of various processes to the Stark width according to the approximative semiclassical approach, we can see that usually dominant contribution to the width of no quenching collisions ($\Delta n=0$) is only 0.224 Å at 20,000 K for the multiplet 7.33. For the same multiplet, the contribution of inelastic collisions ($\Delta n\neq 0$) is 0.329 Å and the correction for strong collisions and higher order multipole interactions 0.400 Å, at the same conditions. From the above analysis one can conclude that the semi-empirical Gaunt factor is not sufficiently large to compensate for the strong collision and higher order multipole interaction yield to the width.

A part of the disagreement between experimental data and the modified semi-empirical approach for the 7.26 and 7.33 multiplets is due also to the failure of the Bates and Damgaard (1949) approach. Strong configuration interaction effects occur in the atomic structure for Si II: they perturb the dipole line strengths; especially in the cases for which an electron of the internal shell $3s^2$ is excited (cf. Nussbaumer, 1977). Finally, the upper levels of these multiplets are autoionization levels: the autoionization widths (w_a) can be large (cf. Artru et al., 1981), and must be added to the collisional width (w_c) before comparing to the experimental one, especially at low densities. For example the width of the line 4190.72 Å has been measured (Kusch and Schröder, 1982) at $N_e=0.5-2\,10^{17}\,\mathrm{cm}^{-3}$. The collisional width is 0.218–0.870 Å and the autoionization width is 0.028 Å (Artru et al., 1981). Since the autoionization width does not depend on electron density, we can see that at $N_e=10^{16}\,\mathrm{cm}^{-3}$, w_a has the same order of magnitude as w_c. It is interesting that in the Si II spectrum transitions exist with $w_a \gg w_c$ at $N_e=10^{17}\,\mathrm{cm}^{-3}$ (e.g. for the level $4p'^2D$ the autoionization width is 150 meV and for $3d'^2F^0$, 409 meV; Artru et al., 1981). Also, autoionization widths within a multiplet may differ several times due to departure from LS coupling. This is an additional reason for eventual differences of experimental line widths within a multiplet.

Table 3. Experimental and theoretical Stark widths (FWHM) of Si III. Experimental data: W_{PDLC}: Purić et al. (1974); W_{PDKP}: Platiša et al. (1977); W_{KS}: Kusch and Schröder (1982). Theoretical data: W_{SEM}: Modified semi-empirical approach. Present calculations and results from Dimitrijević and Konjević (1980, 1981a). W_{SE}: Semi-empirical calculations according to Griem (1968). Results from Dimitrijević and Konjević (1980, 1981a). W_{ASC}: Approximative semi-classical approach. Present calculations and results from Dimitrijević and Konjević (1980, 1981a)

Ion	Transition (multiplet)	Wavelength	T(K)	Experimental data (Å)			Theoretical data (Å)		
				W_{PDLC}	W_{PDKP}	W_{KS}	W_{SEM}	W_{SE}	W_{ASC}
SiIII	$4s^3S$-$4p^3P^o$ (2)	4552.62	8700	0.48			0.778	0.469	0.636
			10600	0.42			0.704	0.424	0.588
			12800	0.40			0.641	0.386	0.548
			16400	0.38			0.566	0.341	0.503
			25600		0.310		0.453	0.272	0.437
		4567.82	8700	0.56			0.778	0.469	0.636
			25600		0.312		0.453	0.272	0.437
		4574.76	23500			3.056	0.469	0.283	0.447
			25600		0.303		0.453	0.272	0.437
SiIII	$4s^1S$-$4p^1P^o$ (4)	5739.73	23500			0.710	0.804	0.495	0.774
SiIII	$4p^3P^o$-$4d^3D$ (5)	3806.54	23500			0.472	0.512	0.343	0.562
		3796.11	23500			0.476	0.512	0.343	0.562
		3791.41	23500			0.376	0.512	0.343	0.562
			25600		0.352		0.490	0.338	0.548
SiIII	$4p^1P^o$-$4d^1D$ (7)	3590.47	23500			0.537	0.664	-	0.688
SiIII	$4p^3P^o$-$5s^3S$ (6)	3241.61	25600		0.321		0.522	0.316	0.526
		3233.95	25600		0.321		0.522	0.316	0.526
		3230.50	25600		0.314		0.522	0.316	0.526
SiIII	$4d^3D$-$5f^3F^o$ (8.06)	3486.91	12800	0.52			3.11*		2.64*

*The line is not isolated

It will be very interesting to obtain reliable experimental data for multiplets 7.26 and 7.33 at various temperatures, since the complex perturbing energy levels structure provides the opportunity to test various approximations within the perturbation – semi-classical formalism.

The experimental and theoretical Stark widths for Si III lines are presented in Table 3. We can see that difference between the various data is within the tolerable limits in all cases with the exception of two values. One of them is the experimental Stark width of Kusch and Schröder for 4574.76 Å line (Mult. 2) approximatively one order of magnitude larger than other experimental and theoretical data (probably a typing error for the order of magnitude?). The other uncertain value is the Stark width for 3486.91 Å (Mult. 8.06) line (Purić et al., 1974). In this case, the perturbing level $5g^3G$ is so close to the $5f^3F^0$ energy level ($32\,cm^{-1}$) that the considered line is not isolated at electron densities of experiment. If we compare the reliable data with calculated values we can se that an average ratio of measured and calculated widths is 0.71 for the modified semi-empirical 1.13 for the semi-empirical and 0.73 for the approximative semi-classical approach.

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