Contrib. Astron. Obs. Skalnaté Pleso **52/3**, 35 – 43, (2022)
https://doi.org/10.31577/caosp.2022.52.3.35

On the Stark broadening parameters of Sn III spectral lines

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Received: August 23, 2022; Accepted: October 5, 2022

Abstract. Stark broadening parameters for four Sn III spectral line obtained by using semiclassical perturbation approach and Stark widths for this transitions obtained by using modified semiempirical approach have been compared with available experimental and semiempirical data and used for the consideration of the influence of the Stark broadening effect in A type stellar atmospheres.

Key words: Atomic data – Spectral lines – A type stars

1. Introduction

Data on Stark broadening are necessary for the study of astrophysical and technological plasmas, and the need for them has also increased in the laboratory and for fusion and lasers. Today, their application in spectroscopy is necessary for a better understanding of the spectrum of an element that is only present in traces in stars.

One of the first report made by Lunt (1907), announces that a strong tin line occured on the ultraviolet side of the iron line in the spectrum of α Scorpii. Some spectral lines of tin have been specifically measured such as 4525.01Å which shows that it is more likely to coincide with Rowland‘s solar line 4525.009Å than with the line closer to the iron line 4525.110Å with different intensities of these two lines. It was also found that many of the tin lines occur in the longer wavelength region.

Tin is an element in Group 14 (the carbon family) and has mainly metallic properties. It has atomic number 50 and an atomic mass of 118.710 atomic mass units. Its ground state electron configuration is noted with [Kr] $4d^{10}5s^25p^2$. Its presence in stellar atmospheres has been reported several times, for example neutral tin in the spectra of A type star γ Equ (Adelman et al., 1979) single ionized tin in Przybylski‘s star by Cowley et al. (2000). Spectral lines of Sn III registered in the NIST database reach the number of 259, most of which have a relative intensity below 500, while the others have a higher intensity of up to 1000. Considering that these lines are of similar intensity and appear often with iron lines, they are often obscured by other lines and for now, they are still difficult to be seen in stellar spectra. Chayer et al. (2005) report the presence of elements beyond the iron group in the atmospheres of the cool DO white dwarfs HD 149499 B and HZ 21, specially Sn IV.

Kieft et al. (2004) measured Stark widths and they also, obtained the first theoretical result by using semiempirical (Griem, 1968) approach. We used this results and compared them with our results for Sn III 6s $^1\mathrm{S}_0 - 6\mathrm{p}\ ^1\mathrm{P}^o_1$ spectral line (Simić et al., 2008). Here we add the following three spectral lines that are compared with experimental and semi-empirical calculations.

Alonso-Medina & Colón (2011) report on the calculated values of the Stark broadening parameters for 171 lines of Sn III arising from $4d^{10}5sns$ $(n = 69)$, $4d^{10}5snp$ $(n = 5, 6), 4d^{10}5p^2, 4d^{10}5snd$ $(n = 57), 4d^{10}5s4f$ and $4d^{10}5s5g$. Stark widths and shifts are presented for an electron density of $10^{23}m^{-3}$ and temperature range (11 00075 000) K. These have been calculated using a semi-empirical approach, with a set of wavefunctions obtained from HartreeFock relativistic calculations, including core polarization effects. The results obtained have been compared with available experimental data.

2. Method

Stark broadening parameter values for doubly charged tin have been obtained using semi-classical method (Sahal-Bréchot, 1969a,b), which is more accurate in contrast to the modified semiempirical method (Dimitrijević & Konjević, 1980) that served us to determine the Stark widths for the same transition thus enabling the comparison of these methods. Different later inovations and optimizations of this theoretical method have been described in details in Sahal-Bréchot (1974, 1991); Fleurier et al. (1977); Dimitrijević et al. (1991); Sahal-Bréchot et al. (2014). Within this theory the FWHM - Full Width at Half intensity Maximum (W) and the shift (d) of an isolated line, originating from the transition between the initial level i and the final level f is expressed for an ionized atom as:

$$W = N \int v f(v) dv \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el} \right)$$

$$d = N \int v f(v) dv \int_{R_3}^{R_D} 2\pi \rho d\rho \sin(2\varphi_p). \qquad (1)$$

where i' and f' are perturbing levels, N and v are the electron density and the velocity of perturbers respectively, $f(v)$ is the Maxwellian distribution of electron velocities, and ρ the impact parameter of the free electron colliding with the emitter.

The inelastic cross sections $\sigma_{ii'}(\upsilon)$ (respectively $\sigma_{ff'}(\upsilon)$), can be expressed by an integration of the transition probability $P_{jj'}(\rho,\upsilon), j = i, f; j' = i', f'$, over the impact parameter ρ as:

$$\sum_{i'\neq i} \sigma_{ii'}(\upsilon) = \frac{1}{2}\pi R_1^2 + \int_{R_1}^{R_D} 2\pi\rho d\rho \sum_{i'\neq i} P_{ii'}(\rho,\upsilon). \tag{2}$$

and the elastic contribution to the width is given by:

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi\rho d\rho \sin^2\delta + \sigma_r,$$
$$\delta = (\varphi_p^2 + \varphi_q^2)^{\frac{1}{2}}. \tag{3}$$

Here σ_{el} is the elastic cross section, while φ_p (r^{-4}) and φ_q (r^{-3}), are phase shifts due to the polarization and quadrupolar potential respectively, and are defined in Section 3 of Chapter 2 in Sahal-Bréchot (1969a). The cut-offs R_1, R_2, R_3, and the Debye radius R_D, as well as the symmetrization procedure are described in Section 1 of Chapter 3 in Sahal-Bréchot (1969b). The contribution of Feshbach resonances, σ_r is explained in Fleurier et al. (1977) and Sahal-Bréchot (2021).

Within the semiclassical perturbation theory is assumed that electrons are moving along hyperbolic paths due to attractive Coulomb force, while in the case of ionic perturbers this force is repulsive, so that trajectories are different. For ion-impact broadening the formulae are analogous to Eqs. (1) - (3) for electron-impact broadening.

If the considered lines are isolated, the line profile $F(\omega)$ has Lorentzian form and can be expressed as:

$$F(\omega) = \frac{W/(2\pi)}{(\omega - \omega_{if} - d)^2 + (W/2)^2} \tag{4}$$

where

$$\omega_{if} = \frac{E_i - E_f}{\hbar}$$

and E_i, E_f are the energies of initial and final state, respectively. Consequently, if we know Stark width W and shift d it is easy to determine the profile of a considered spectral line.

In addition to the semiclassical method, we also performed a calculation using a modified semiempirical method (MSE) which is described in details in reference Dimitrijević & Konjević (1980).

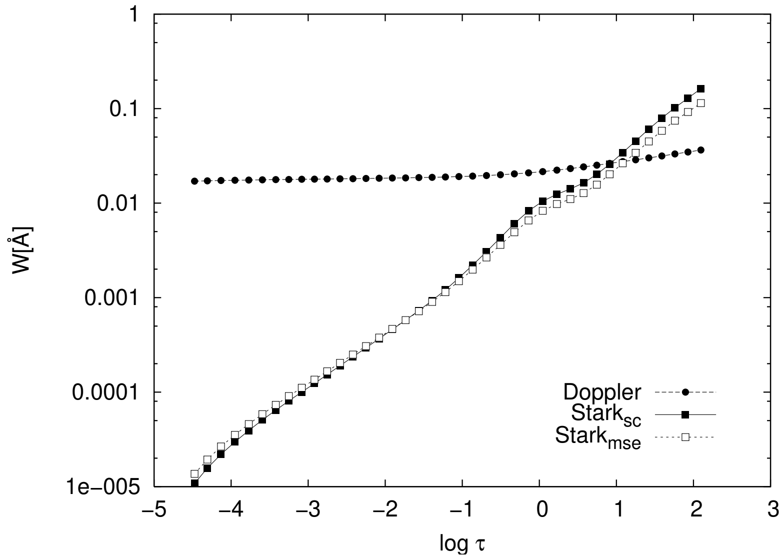

Figure 1. Stark widths (sc-semiclasical and mse-modified semiempirical) and thermal Doppler widths for Sn III 5226.2 Å spectral lines as a function of Roseland optical depth for an A type model of stellar atmosphere $T_{\rm eff} = 10000$ K, $\log g = 4.5$ (Kuruczs, 1979).

3. Results

For four doubly ionized tin spectral lines Stark broadening parameters, the full semiclassical perturbation approach (Sahal-Bréchot, 1969a,b) as well as the modified semiempirical approach (Dimitrijević & Konjević, 1980) have been applied. The needed energy levels have been taken from Moore (1971). The oscillator strengths have been calculated by using the method of Bates & Damgaard (1949), and the tables of Oertel & Shomo (1968). For higher levels, the method of van Regemorter et al. (1979) has been used.

The tables 1 and 2 contain the results of our calculations of Stark broadening parameters for four lines of Sn III and we specify a parameter C (Dimitrijević & Sahal-Bréchot, 1984) which gives an estimate for the maximum perturber density for which the line may be treated as isolated, when it is divided by the corresponding full width at half maximum.

Experimental values by Kieft et al. (2004) have been obtained by arc discharge through tin vapor. The Stark half-widths of doubly ionized tin have been measured at an electron density of 10^{17}cm^{-3} and an electron temperature of 11604 K. All broadening mechanisms have been investigated. Natural broadening is negligible. The Doppler broadening only becomes significant at 30 times higher electron temperature values, but does not exceed the value

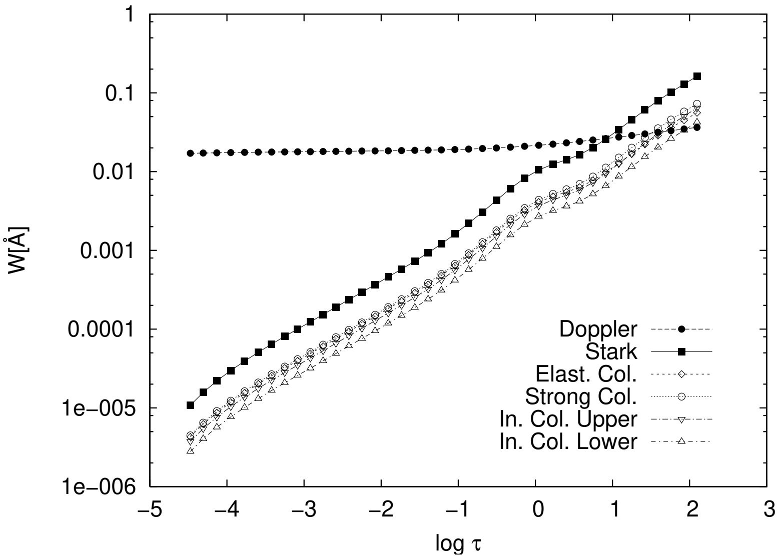

Figure 2. Stark and thermal Doppler widths and widths due to various collisional processes for Sn III 5226.2 Å spectral lines as a function of Roseland optical depth for an A type model of stellar atmosphere $\mathrm{T_{eff}} = 10000$ K, $\log g = 4.5$ Kuruczs (1979).

of 0.25Å. Broadening due to collisions with neutral atoms is far less than the interaction with charged particles. Therefore, Stark broadening dominates all the mentioned mechanisms. All measured Sn III profiles show a Voight profile, with a fixed Gaussian contribution originating in the aperture profile while the Lorentzian contribution is entirely attributed to Stark broadening.

Experimental and theoretical values within the framework of semi-empirical approaches obtained by Kieft et al. (2004) for spectral lines Sn III for which we also did the calculations enable us to compare the obtained results. There is a good agreement with experimental value of both our results obtained by using semiclassical and modified semiempirical approach for Stark width for Sn III, see Table 3. Obviously, this ratio is better for our values than for semiempirical one obtained by Kieft et al. (2004) using Griem (1968) method, which uses semiempirical Gaunt factor suitable for singly charged ions (see Dimitrijević & Konjević, 1980).

We used Kuruczs (1979) atmosphere model of A type star with effective temperature $\mathrm{T_{eff}} = 10000$ K and logarithm of surface gravity $\log g = 4.5$. As one can see from Fig 1. there are layers where Stark broadening is less significant compared to the thermal Doppler effect, but, if it is not sufficiently small, it may have influence on the wings of the spectral line. For $\log \tau \geq 1$ Stark broadening effect is more and more expressive and becomes the dominant. Contributions of

Table 1. Stark broadening parameters for Sn III spectral lines for perturber density of 10^{17}cm^{-3} and temerature range from 10000 up to 150000 K, obtained by using the semiclassical perturbation method (Sahal-Bréchot, 1969a,b)

Transition	T (K)	W_e (Å)	d_e (Å)	W_p (Å)	d_p (Å)	$W_{He^{++}}$ (Å)	$d_{He^{++}}$ (Å)
	10000	1.39	-0.149	0.391E-01	-0.207E-01	0.507E-01	-0.189E-01
Sn III	20000	1.05	-0.987E-01	0.615E-01	-0.339E-01	0.724E-01	-0.294E-01
6s $^1S_0 - 6p\ ^1P^o_1$	30000	0.907	-0.886E-01	0.758E-01	-0.426E-01	0.794E-01	-0.361E-01
5226.2 Å	50000	0.788	-0.900E-01	0.869E-01	-0.513E-01	0.891E-01	-0.423E-01
C= 0.24E+21	100000	0.676	-0.846E-01	0.102	-0.619E-01	0.101	-0.505E-01
	150000	0.626	-0.788E-01	0.111	-0.686E-01	0.106	-0.557E-01
	10000	0.921	0.727E-02	0.338E-01	0.340E-02	0.460E-01	0.332E-02
Sn III	20000	0.692	0.121E-01	0.526E-01	0.673E-02	0.648E-01	0.619E-02
5d $^3D_1 - 6p\ ^3P^o_1$	30000	0.594	0.122E-01	0.640E-01	0.919E-02	0.712E-01	0.806E-02
5292.7 Å	50000	0.504	0.143E-01	0.722E-01	0.119E-01	0.783E-01	0.104E-01
C= 0.52E+21	100000	0.423	0.147E-01	0.817E-01	0.159E-01	0.871E-01	0.130E-01
	150000	0.389	0.155E-01	0.870E-01	0.177E-01	0.902E-01	0.144E-01
	10000	0.945	0.786E-02	0.347E-01	0.358E-02	0.471E-01	0.349E-02
Sn III	20000	0.710	0.128E-01	0.539E-01	0.707E-02	0.664E-01	0.650E-02
5d $^3D_2 - 6p\ ^3P^o_1$	30000	0.610	0.129E-01	0.656E-01	0.964E-02	0.730E-01	0.843E-02
5350.7 Å	50000	0.517	0.150E-01	0.740E-01	0.125E-01	0.802E-01	0.109E-01
C= 0.53E+21	100000	0.434	0.155E-01	0.838E-01	0.166E-01	0.892E-01	0.135E-01
	150000	0.399	0.163E-01	0.891E-01	0.185E-01	0.924E-01	0.151E-01
	10000	0.948	0.791E-02	0.347E-01	0.371E-02	0.471E-01	0.361E-02
Sn III	20000	0.712	0.132E-01	0.539E-01	0.730E-02	0.665E-01	0.671E-02
5d $^3D_1 - 6p\ ^3P^o_0$	30000	0.612	0.133E-01	0.656E-01	0.995E-02	0.731E-01	0.868E-02
5371.1 Å	50000	0.519	0.154E-01	0.741E-01	0.129E-01	0.803E-01	0.112E-01
C= 0.53E+21	100000	0.434	0.172E-01	0.839E-01	0.170E-01	0.894E-01	0.140E-01
	150000	0.399	0.167E-01	0.892E-01	0.190E-01	0.925E-01	0.155E-01

different collision processes to the total Stark width in comparison with Doppler one, can be seen in Fig. 2. The behavior with log τ is similar for Full Stark width as well as for strong, elastic, upper and lower level inelastic contributions..

The investigated Stark broadening parameters for the Sn III are of importance for the study of astrophysical and technological plasmas. For the four selected lines a comparison between semi-classical method Sahal-Bréchot (1969a,b) and the modified semi-empirical method Dimitrijević & Konjević (1980) is carried out. The more precise, but also more time consuming semiclassical method and MSE have shown a good agreement of the calculated data. The importance of the Stark broadening processes is analyzed with the help of the Kuruczs (1979) model. From the presented results it could be seen that the use of modified semiempirical method is valid for the analyzed lines and as such could be a recommended one for the fast calculations for the broadening parameters within the ranges of investigated plasma conditions. There is a need for further investigation of lines that could be observed in stellar and laboratory plasma, and as such it is still an open field for both theoretical as well as experimental research and observations.

Table 2. Stark widths obtained by MSE method (Dimitrijević & Konjević, 1980) for Sn III spectral lines for perturber density of $10^{17}\mathrm{cm}^{-3}$ and temperature range from 2500 do 50000 K. These values have been calculated separately in order to compare with the semiclassical results. Only for Sn III 6s $^1S_0 - 6p\ ^1P_1^o$ spectral line results are taken from Simić et al. (2008)

Transition	T(K)	W(Å)	Prelaz	T(K)	W(Å)
	2500	2.217		2500	1.497
	5000	1.567		5000	1.059
6s $^1S_0 - 6p\ ^1P_1^o$	10000	1.108	5d $^3D_2 - 6p\ ^3P_1^o$	10000	0.749
5226.2Å	20000	0.784	5350.7Å	20000	0.529
	30000	0.640		30000	0.432
	50000	0.514		50000	0.339
	2500	1.465		2500	1.500
	5000	1.036		5000	1.061
5d $^3D_1 - 6p\ ^3P_1^o$	10000	0.732	5d $^3D_1 - 6p\ ^3P_0^o$	10000	0.750
5292.7Å	20000	0.518	5371.6Å	20000	0.530
	30000	0.423		30000	0.433
	50000	0.332		50000	0.340

Table 3. Comparison between W_m-experimental Stark widhts (Kieft et al., 2004) with theoretical: W_{se}-semiempirical (Kieft et al., 2004), W_{sc}-semiclasical i W_{mse}-modified semiempirical. Results performed for an electron density of $10^{17}\mathrm{cm}^{-3}$ and an electron temperature of 11604K.

Transition	W_m(Å)	Rel. exp error	$\frac{W_m}{W_{se}}$	$\frac{W_m}{W_{sc}}$	$\frac{W_m}{W_{mse}}$
Sn III 6s $^1S_0 - 6p\ ^1P_1^o$ 5226.2 Å	1.22	50%	1.70	0.92	1.15
Sn III 5d $^3D_1 - 6p\ ^3P_1^o$ 5292.7 Å	0.86	30%	1.43	0.98	1.23
Sn III 5d $^3D_2 - 6p\ ^3P_1^o$ 5350.7 Å	0.68	30%	1.13	0.76	0.96
Sn III 5d $^3D_1 - 6p\ ^3P_0^o$ 5371.1 Å	0.64	30%	1.07	0.70	0.90

Acknowledgements. This work is supported by Ministry of Education, Science and Technological Development of the Republic of Serbia through the project contract No. 451-03-68/2022-14/200002 and 451-03-68/2022-14/200024.

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