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On the Stark broadening of some Cr II spectral lines in plasma

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Abstract. New electron-impact line widths for eight Cr II multiplets have been calculated within the modified semiempirical (MSE) approach. Needed energy levels and radial integrals are calculated by different methods. The Stark widths are obtained as a function of temperature, for perturber density of 10^{17} cm^{-3} and have been compared with the approximate formula of Cowley and with recent experimental results. The obtained results are of interest for diagnostic and modeling of laboratory and stellar plasmas. The obtained data will be included in the STARK-B database, which is part of the Virtual Atomic and Molecular Data Center VAMDC.

Key words: Spectral lines – Plasma – Atomic data – Stark broadening

1. Introduction

Chromium in various ionization stages has been observed in the spectra of white dwarf atmospheres, where the Stark broadening is usually dominant broadening mechanism, especially in deeper atmospheric layers (Simić *et al.*, 2006; Hamdi *et al.*, 2008; Dufour *et al.*, 2011; Hamdi *et al.*, 2014; Dimitrijević and Chougule, 2018). In order to determine chromium abundance in such stars, as well as for opacity calculations and more sophysticated stellar atmosphere modeling, we need the corresponding Stark broadening data. Such data are also of interest for laboratory plasma diagnostics and modeling, as well as for investigation of fusion and laser produced plasmas where addition of different impurities may change different plasma parameters.

Nine Cr I spectral line widths, due to Stark broadening, are calculated by Dimitrijević *et al.* (2005). Seven multiplets belonging to 4s-4p transitions of Cr

II spectral lines are calculated by Dimitrijević *et al.* (2007) and nine resonant Cr II multiplets by Simić *et al.* (2013). Stark spectral line widths of six Cr III transitions are calculated by Dimitrijević and Chougule (2018). Cr VI spectral line widths for two multiplets are calculated by Dimitrijević *et al.* (2017). In this work, in order to provide new Stark broadening data for stellar and laboratory plasma research, we calculate Stark spectral line widths for eight Cr II multiplets for an electron density of 10^{17} cm^{-3} and a range of temperature between 5 000 K and 50 000 K. The obtained results will be in STARK-B database (http://stark-b.obspm.fr/, Sahal-Bréchot *et al.* (2015)) which is included in Virtual Atomic and Molecular Data Center (VAMDC Consortium http://vamdc.org Dubernet *et al.* (2016), Moreau *et al.* (2018)).

2. Method of calculations

The modified semiempirical approach (MSE) by Dimitrijević and Konjević (1980) has its origin from the semiempirical approach (SE) by Griem (1968) where Stark widths are calculated as a function of inelastic cross sections for the emitter collisions with perturbers, expressed using the empirical Gaunt factors $g(x)$, within the impact approximation taking into account the elastic collisions approximately, by extrapolation of Gaunt factors below the threshold for inelastic collisions:

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

where $\Delta E = |E - E_j|$.

In the MSE approach (Dimitrijević and Konjević, 1980) a modified Gaunt factors $\tilde{g}(x) = 0.7 - \frac{1.1}{Z} + g(x)$ is used for Δn = 0:

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

where $Z-1$ is the ionic charge and n_i^* and n_f^* are the effective principal quantum numbers of initial and final transition level respectively (in its original form, the spectral line width depends only on the upper principal quantum number). The effective principal quantum number n_j^* is related by the energy level E_j as:

$$\left(n_j^*\right)^2 = Z^2\frac{E_H}{E_{ion} - E_j} \tag{3}$$

where E_H is the hydrogen atom energy.

Energy levels needed in our MSE calculations are taken from the NIST database (Kramida *et al.*, 2018), oscillator strengths were calculated using the method of Bates and Damgaard (1949) and tables of Oertel and Shomo (1968). For higher levels, the method described in van Regemorter *et al.* (1979) was applied.

The MSE is valid for singly and multicharged ions and the number of input atomic data is minimized. In the MSE approach, only the matrix elements of transitions with Δn = 0 should be calculated, while other transitions are separated and grouped together. The advantage of this method is that smaller number of atomic data is needed for calculation than the more sophisticated calculations in semiclassical perturbation (SCP) ones (Sahal-Bréchot et al., 2014). Accuracy of MSE results is usually within an error bars of $\pm$ 50 percent.

The Cowley formula (Cowley, 1971) was used extensively in astrophysics, for example it was used by Majlinger et al. (2017):

$$W_{Cowley} = N \frac{\pi}{c} \frac{\hbar^2}{m^2} \left(\frac{2m}{\pi k T} \right)^{1/2} \frac{\lambda^2}{Z^2} \left[(n_i^*)^4 + (n_f^*)^4 \right] \tag{4}$$

where λ is the wavelength of the line.

3. Results and discussion

We evaluated Stark widths using the MSE approach for 8 selected Cr II spectral lines. The Stark widths are calculated for an electron density of 10^{17} cm^{-3}, which is usually used in tables for ion emitters, and for different temperature values. To make the usage of obtained results for modelisation of stellar atmospheres and spectra easier, as well as for radiative transfer calculations, and to prepare our results for the implementation in the STARK-B database, we used the formula from Sahal-Bréchot et al. (2011) for fitting calculated data within the range 5 000 K 50 000 K with temperature:

$$\log(W) = a_0 + a_1 \log(T) + a_2 \log^2(T) \tag{5}$$

where, W is the FWHM Stark width in Å, T is the temperature in Kelvin and a_0, a_1 and a_2 are the fitting parameters obtained for electron density of 10^{17} cm^{-3}.

Stark width (FWHM) values for temperatures from 5 000 K to 50 000 K are given in Table 1, since this temperature interval is interesting for plasma diagnostic of white dwarf atmospheres and laser produced plasmas.

In this Table 1, W_{MSE} is our calculated Stark width using the MSE approach (Equation 1) and W_{Cowley} using Equation 4. The wavelengths in Table 1 are calculated from the corresponding energy levels given as the input so that they may differ from the observed ones.

We give in Table 2, the fitting parameters a_0, a_1 and a_2 with the R correlation coefficient in %.

Table 1. Stark electron-impact widths (full widths at half maximum, FWHM) for Cr II spectral lines:W_{MSE}, calculated by using the modified semiempirical (MSE) method; W_{Cowley}, calculated by using the approximate formula of Cowley. The temperatures are from 5000 K up to 50000 K and the electron density is 10^{17} cm^{-3}.

Transition	Temp.	W_{MSE}	W_{Cowley}
Cr II $3d^4(a^1G)4s^2P$ - $3d^4(a^1G)4p^2P^o$	5000	1.58E-01	1.65E-01
	10000	1.12E-01	1.17E-01
3172.07 Å	20000	7.92E-02	8.26E-02
3kT/2ΔE= 0.349	30000	6.47E-02	6.75E-02
	50000	5.01E-02	5.23E-02
Cr II $3d^4(a^3F)4s^2F$ - $3d^4(a^3F)4p^2F^o$	5000	1.43E-01	152E-01
	10000	1.01E-01	1.08E-01
3028.12 Å	20000	7.16E-02	7.62E-02
3kT/2ΔE= 1.14	30000	5.84E-02	6.22E-02
	50000	4.53E-02	4.82E-02
Cr II $3d^4(^3G)4s^2G$ - $3d^4(^3G)4p^2G^o$	5000	1.55E-01	1.65E-01
	10000	1.09E-01	1.17E-01
3107.56 Å	20000	7.73E-02	8.27E-02
3kT/2ΔE= 0.327	30000	6.31E-02	6.75E-02
	50000	4.89E-02	5.23E-02
Cr II $3d^4(a^1G)4s^2G$ - $3d^4(a^1G)4p^2G^o$	5000	1.17E-01	1.27E-01
	10000	8.24E-02	9.01E-02
2777.27 Å	20000	5.83E-02	6.37E-02
3kT/2ΔE= 0.302	30000	4.76E-02	5.20E-02
	50000	3.69E-02	4.03E-02
Cr II $3d^4(a^3P)4s^4P$ - $3d^4(a^3P)4p^4D^o$	5000	1.26E-01	1.34E-01
	10000	8.92E-02	9.47E-02
2943.75 Å	20000	6.31E-02	6.69E-02
3kT/2ΔE= 0.307	30000	5.15E-02	5.47E-02
	50000	3.99E-02	4.23E-02
Cr II $3d^4(^3H)4s^4H$ - $3d^4(^3H)4p^4H^o$	5000	1.28E-01	1.36E-01
	10000	9.07E-02	9.61E-02
2981.09 Å	20000	6.41E-02	6.80E-02
3kT/2ΔE= 0.311	30000	5.24E-02	5.55E-02
	50000	4.06E-02	4.30E-02
Cr II $3d^4(^3D)4s^4D$ - $3d^4(^3D)4p^4D^o$	5000	1.17E-01	1.26E-01
	10000	8.28E-02	8.92E-02
2846.26 Å	20000	5.85E-02	6.31E-02
3kT/2ΔE= 0.297	30000	4.78E-02	5.15E-02
	50000	3.70E-02	3.99E-02
Cr II $3d^4(^5D)4s^6D$ - $3d^4(^5D)4p^6F^o$	5000	1.17E-01	1.26E-01
	10000	8.26E-02	8.89E-02
2850.70 Å	20000	5.84E-02	6.29E-02
3kT/2ΔE= 0.297	30000	4.77E-02	5.13E-02
	50000	3.70E-02	3.98E-02

Table 2. Fitting parameters for approximate formula (5). R^2(%) is the square of the correlation coefficient.

Transition	λ(Å)	a_0	a_1	a_2	R^2(%)
$3d^4(a^1G)4s^2P$ - $3d^4(a^1G)4p^2P^o$	3172.07	1.00340	-0.47920	-0.00235	0.9999976
$3d^4(a^3F)4s^2F$ - $3d^4(a^3F)4p^2F^o$	3028.12	1.02325	-0.50967	0.00126	0.9999966
$3d^4(^3G)4s^2G$ - $3d^4(^3G)4p^2G^o$	3107.56	1.12564	-0.54132	0.00487	0.9999823
$3d^4(a^1G)4s^2G$ - $3d^4(a^1G)4p^2G^o$	2777.27	0.99869	-0.53851	0.00448	0.9999913
$3d^4(a^3P)4s^4P$ - $3d^4(a^3P)4p^4D^o$	2943.75	0.92591	-0.48882	-0.00127	0.9999993
$3d^4(^3H)4s^4H$ - $3d^4(^3H)4p^4H^o$	2981.09	0.93937	-0.49250	-0.00075	0.9999985
$3d^4(^3D)4s^4D$ - $3d^4(^3D)4p^4D^o$	2846.26	0.90349	-0.49312	-0.00082	0.9999991
$3d^4(^5D)4s^6D$ - $3d^4(^5D)4p^6F^o$	2850.70	0.97414	-0.52729	0.00325	0.9999963

We compared in Table 3 our results with those obtained experimentally by Aguilera *et al.* (2014). For spectral line widths within a multiplet, we used the formula:

$$W_{line} = \left(\frac{\lambda_{line}}{\lambda_{Mult}}\right)^2 W_{Mult} \tag{6}$$

where W_{line} and λ_{line} are for the particular line within the multiplet; W_{Mult} and λ_{Mult} are the values for the multiplet.

Table 3. Comparison of our MSE Stark width calculations W_{MSE} with experimental widths W_{Agl} from Aguilera *et al.* (2014). Lines are sorted by wavelength.

Transition	Multiplet	λ(Å)	W_{Agl}	W_{MSE}	$\frac{W_{Agl}}{W_{MSE}}$
$3d^4(a\ ^1G)4s$ - $3d^4(a\ ^1G)4p$	c ^2G w $^2G^o$	2774.43	6.96E-02	6.30E-02	0.91
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2835.63	6.91E-02	5.00E-02	0.72
$3d^4(^3D)4s$ - $3d^4(^3D)4p$	c ^4D w $^4D^o$	2838.78	6.41E-02	5.50E-02	0.86
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2843.25	6.94E-02	5.10E-02	0.73
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2849.83	6.98E-02	5.10E-02	0.73
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2855.67	7.00E-02	5.00E-02	0.71
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2860.93	7.03E-02	5.00E-02	0.71
$3d^4(^5D)4s$ - $3d^4(^5D)4p$	a ^6D z $^6F^o$	2862.57	7.04E-02	4.70E-02	0.67
$3d^4(^3G)4s$ - $3d^4(^3G)4p$	b ^2G x $^2G^o$	2927.08	8.27E-02	7.90E-02	0.96
$3d^4(^3P)4s$ - $3d^4(a\ ^3P)4p$	b ^4P y $^4D^o$	2930.85	7.50E-02	6.60E-02	0.88
$3d^4(^3P)4s$ - $3d^4(a\ ^3P)4p$	b ^4P y $^4D^o$	2935.13	7.53E-02	6.60E-02	0.88
$3d^4(^3P)4s$ - $3d^4(a\ ^3P)4p$	b ^4P y $^4D^o$	2961.72	7.66E-02	6.20E-02	0.81
$3d^4(^3H)4s$ - $3d^4(^3H)4p$	a ^4H z $^4H^o$	2971.90	7.71E-02	7.10E-02	0.92
$3d^4(^3P)4s$ - $3d^4(a\ ^3P)4p$	b ^4P y $^4D^o$	2976.71	7.74E-02	6.00E-02	0.78
$3d^4(^3H)4s$ - $3d^4(^3H)4p$	a ^4H z $^4H^o$	2979.74	7.75E-02	7.00E-02	0.90
$3d^4(^3H)4s$ - $3d^4(^3H)4p$	a ^4H z $^4H^o$	2989.19	7.80E-02	6.80E-02	0.87
$3d^4(^3F)4s$ - $3d^4(a\ ^3F)4p$	b ^2F z $^2F^o$	3028.12	8.55E-02	7.70E-02	0.90
$3d^4(^3P)4s$ - $3d^4(a\ ^3P)4p$	a ^2P z $^2P^o$	3172.07	9.47E-02	7.80E-02	0.82

We obtain for all the considered lines 0.82 as a mean value of the ratio $\frac{W_{Agl}}{W_{MSE}}$ with a standard deviation of s=0.088, so the calculated values are approximately 20 % higher than the experimental ones.

4. Conclusions

We calculated Stark electron-impact widths using the MSE method for a range of temperatures from 5 000 K to 50 000 K and for an electron density of 10^{17} cm^{-3}. These new eight Cr II Stark widths calculated in this work, for the lines were other theoretical Stark broadening data are missing, are of interest for stellar plasma, laboratory plasma diagnostics, laser produced plasma, as well as for analysis and modeling of stellar atmospheres. An extension of the Stark broadening calculations to other lines of Cr II will be an interesting future work and also applications of the atomic and spectroscopic data of these lines to typical stars where Stark broadening is an important mechanism in their atmospheres.

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