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ON THE STARK BROADENING OF Zr IV IN THE SPECTRA OF DB WHITE DWARFS

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Abstract. The electron-impact widths for four Zr IV spectral lines have been calculated by using the modified semiempirical method. Additionally, by using the obtained results we analized the importance of Stark broadening in the spectra of DB white dwarfs.

1. INTRODUCTION

Zirconium has a significant role in stellar spectroscopy as a member of Sr-Y-Zr triad, important in studying of s-process of nucleosynthesis in HgMn type of so-called chemically peculiar (CP) stars. These stars show great anomalies in their abundances (Lecrone et al, 1993) and provide us a useful informations about stellar evolution. Zirconium is often overabundant in HgMn star spectrum giving thus a better insight in a complex dinamical proccesses occuring in their interior and atmosphere (Heacox, 1979). Also, it is evident (Lecrone et al, 1993, Sikström et al. 1999) that the zirconium abundance determination from weak Zr II optical and from strong Zr III UV spectral lines give significantly different results. This, so-called «zirconium conflict» is still unresolved mistery supposed to be explained as a result of inadequate use of stellar model, e.g. without taking into account of non-LTE effects or diffusion.

The Stark broadening of spectral lines in stellar plasma has already been studied in the case of singly (Zr II) and doubly (Zr III) charged zirconium ions (Popović and Dimitrijević, 1996, 1997, Popović et al. 2001). We hope that new foundings about abundance of triply charged zirconium ions (Zr IV) in stellar spectra get us closer to the solution of «zirconium conflict» mentioned above. Although this problem cannot be solved without the reliable Stark broadening parameters, since it is shown (see for example Popović et al. 2001) that neglecting the Stark effect influence on line width calculation can cause errors in abundance determination.

2. METHOD OF CALCULATION

Here, we provided Stark full width at half maximum (FWHM) for four transitions of Zr IV, calculated using the modified semiempirical method MSE (Dimitrijević and Konjević 1980) of interest not only for in astrophysics, but also for laboratory, and technological plasmas investigations.

Modified semiempirical method (Dimitrijević and Konjević 1980), for the Stark broadening of isolated, nonhydrogenic ion lines, has been described elsewhere (for example, see Dimitrijević and Popović, 2001). Compared to some other approaches for Stark width and shift calculations, such as semiempirical method of Griem (1968) or semiclassical perturbation method of Sahal-Bréchot (1969a,b), MSE needs less atomic data. If there is no perturbing levels violating the assumed approximations, only energy levels with $\Delta n=0$ and orbital quantum numbers l_i , l_f , $l_i \pm 1$, $l_f \pm 1$ (where l_i and l_f represent initial and final orbital quantum numbers of transition respectively) are needed for a line width calculation. All levels with $\Delta n \neq 0$, needed for semiempirical or semiclassical perturbation methods, are lumped together here and approximately estimated, significantly simplifying calculation technique. The needed matrix elements are obtained within the Coulomb approximation formalism of Bates and Damgaard (1949), while the line and multiplet factors are taken from Shore and Menzel (1968) whenever it is neccesary. MSE approach is tested and confirmed many times, even for complex spectra, mostly with an accuracy not worse then ±50% (Dimitrijević and Konjević 1980, Popović and Dimitrijević, 2001).

3. RESULTS AND DISCUSSION

The Stark width calculations for four Zr IV transitions, 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ λ = 2287.38, 5s $^2S_{1/2}$ - 5p $^2P^o_{3/2}$ λ = 2164.36, 5p $^2P^o_{1/2}$ – 5d $^2D_{3/2}$ λ = 1536.67 and 5p $^2P^o_{3/2}$ – 5d $^2D_{3/2}$ λ = 1607.95 have been performed. The energy levels used to calculate electron-impact FWHM of spectral lines have been taken from Reader and Acquista (1997). The Stark widths are calculated for the electron density of 10^{23} m^{-3} and for temperatures from 10000 K to 500000 K.

Table 1. Stark full widths at half maximum (W_{Mse}) for for the electron density of 10^{23} m^{-3} and for temperatures from 10000 K to 500000 K. W_{Pur}(Å), estimates of Purić and Šćepanović (1999).

	T(K)	W_{Mse}(Å)	W_{Pur}(Å)	W_{Mse}/W_{Pur}
Zr IV λ=2287.38Å 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$	10000	0.08435	0.06305	1.34
	20000	0.05964	0.04459	1.34
	50000	0.03772	0.02820	1.34
	100000	0.02704	0.01994	1.36
	200000	0.02154	0.01409	1.53
	300000	0.01997	0.01151	1.74
	500000	0.01048	0.00892	1.17

	T(K)	W_{Mse}(Å)	W_{Pur}(Å)	W_{Mse}/W_{Pur}
Zr IV λ=2164.36Å 5s $^2S_{1/2}$ - 5p $^2P^o_{3/2}$	10000	0.07681	0.05645	1.36
	20000	0.05431	0.03992	1.36
	50000	0.03435	0.02525	1.36
	100000	0.02457	0.01785	1.38
	200000	0.01959	0.01262	1.55
	300000	0.01811	0.01031	1.76
	500000	0.01702	0.00798	2.13

	T(K)	W_{Mse}(Å)	W_{Pur}(Å)	W_{Mse}/W_{Pur}
Zr IV λ = 1536.67Å 5p $^2P^o_{1/2}$ – 5d $^2D_{3/2}$	10000	0.04218	0.05318	0.79
	20000	0.02983	0.03760	0.79
	50000	0.01887	0.02378	0.79
	100000	0.01341	0.01682	0.80
	200000	0.01064	0.01189	0.89
	300000	0.01011	0.00971	1.04
	500000	0.01005	0.00752	1.33

Zr IV $\lambda = 1607.95$Å 5p $^2P^o_{3/2} - 5d\ ^2D_{3/2}$	T(K)	W_{Mse}(Å)	W_{Pur}(Å)	W_{Mse}/W_{Pur}
	10000	0.04690	0.06058	0.77
	20000	0.03316	0.04284	0.77
	50000	0.02097	0.02709	0.77
	100000	0.01488	0.01916	0.78
	200000	0.01181	0.01355	0.87
	300000	0.01120	0.01106	1.01
	500000	0.01115	0.00857	1.30

We compared our results with estimates of Purić and Šćepanović (1999). The equation obtained from Purić's regression analysis of existing set of Stark broadening data for all ionisation levels of the multiply charged ions and for all elements along the periodic table was adopted for our purpose. After transformation of width from Purić and Šćepanović (1999), which are in angular frequency units, in Å (see for example Dimitrijević and Konjević, 1984) the Stark width is:

$$W_{Pur} = a \cdot Z^{c} \cdot \lambda^{2} \cdot N \cdot T^{-1/2} \cdot (E_{ion}-E_f)^{-b}$$

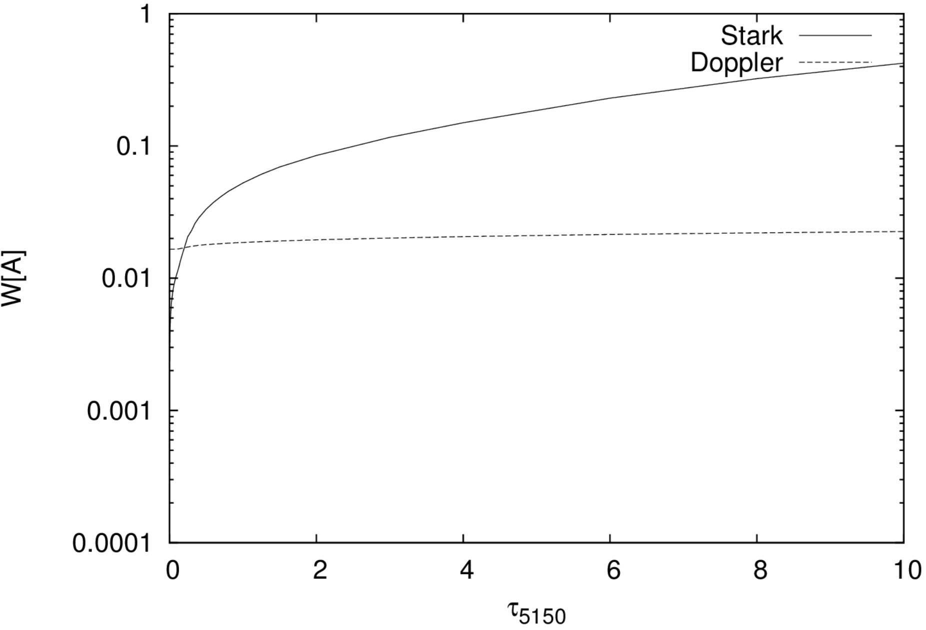

Figure 1. Thermal Doppler and Stark widths for Zr IV 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ λ = 2287.38 Å spectral line for a DB white dwarf atmosphere model with T_{eff} = 15,000 K and log g = 8, as a function of optical depth τ_{5150}.

where W_{Pur} is the estimated width of Purić and Šćepanović (1999) in Å, λ spectral line wavelenght in Å, E_{ion} and E_f energies of ionization and of final level of transition in eV respectively, T temperature in K, Z rest core charge and N electron density in m^{-3}. Coefficients a , b and c are independent of temperature, ionization potential and electron density for a given transition. Coefficients values are $a = 3.27 \cdot 10^{-28}$, $b = 3{,}1$ and $c = 5.2$ (according to Purić and Šćepanović, 1999). The tabulated results show a very good agreement. It is interesting that ratio between calculated and estimated widths remains equal for the temperatures below 100000 K, but above this limit accuracy becomes worst. This phenomenon could be a consequence of approximate use of temperature dependence in the formula of Purić and Šćepanović (1999).

We tested our results in stellar plasma conditions of DB white dwarf atmosphere. White dwarfs have a strong gravity field intensity on their surface causing that the change of particle density being more rapide with the depth then in some other stellar objects. We note also, that Stark width shows linear correlation with the plasma concentration, and Doppler width depends on temperature only. One can see in Fig. 1 that the Stark width is dominant in comparison with Doppler width in DB dwarf stellar spectra, as it has been proved in some recent investigations (see e.g. Simić et al. 2006). For this comparison, the existing stellar model atmosphere for DB white dwarfs published by Wickramasinghe (1972) is taken with log $g = 8$ and $T_{eff} = 15000$ K.

It is evident from the Figure 1 that the electron-impact width shows the significant dependence on the optical depth in the atmosphere of DB white dwarf, while the thermal width almost remains constant with the optical depth change, and that Stark broadening is dominant in comparison with Doppler broadening.

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