Publ. Astron. Obs. Belgrade No. 96 (2017), 133 - 139 *Contributed Paper*

SPECTRAL LINES OF Zr IV IN THE ATMOSPHERE OF CHEMICALLY PECULIAR STARS

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Abstract. The electron-impact widths for seven Zr IV spectral lines have been calculated by using the modified semi-empirical method. With obtained results, the importance of Stark broadening in the spectra of DB white dwarfs has been analysed.

1. INTRODUCTION

Stark broadening is usually the main pressure broadening mechanism for spectral lines from white dwarf and hot star atmospheres of earlier spectral types. Some of these stars, so-called *Chemically Peculiar Stars* (CP), show great anomalies in their abundances (see e.g. Leckrone et al, 1993), e.g. some elements are over- or underabundant compared with the solar ones. About 10-20 percent of A and B stars are classified as CP stars according to their physical characteristics and they can be found mostly in the upper quarter of Main-Sequence of the H-R diagram. Regarding the fact that we consider early-type stars younger than Sun, some of CP stars can provide us useful informations about early stage of stellar evolution.

A typical representative member of a non-magnetic subclass HgMn CP stars is a spectroscopic binary χ Lupi. Except Hg and Mn, Zr is also found overabundant in this double star. Zirconium has an important place in stellar spectroscopy investigations as a member of Sr-Y-Zr triad, appearing in s-process nucleosynthesis scenario. The Stark broadening of spectral lines of singly (Zr II) and doubly (Zr III) charged zirconium ion in stellar plasma has been investigated in the earlier researches (Popović and Dimitrijević 1996,1997, Popović et al 2001), especially related to the attempt to clarify the so-called "zirconium conflict". Namely, the zirconium abundance values determined from weak Zr II optical and from strong Zr III UV spectral lines of χ Lupi differ from each other more then an order of magnitude (Leckrone et al, 1993, Sikström et al 1999). This strange result can be justified with inadequate use of stellar model, some non-LTE effect or radiative diffusion mechanism, but further researches in this case are needed. In spite of binary nature of χ Lupi, zirconium conflict also can be explained by some unknown interaction process between two stellar components. A better knowledge of Stark broadening is also of interest for the better understanding of this problem. In addition to the Stark broadening data for Zr II and Zr III spectral lines, it is of interest to also provide Stark width of triply-ionized zirconium (Zr IV) spectral lines, since they could be important for its abundance determination, avoiding the Zr II and Zr III lines for which the zirconium conflict has been established. Moreover, it has been already shown that the neglecting of the Stark broadening could lead to wrong values of abundances (Popović et al 2001).

Another type of celestial objects interesting for our investigation of Stark broadening are white dwarfs. In their case, not only the effective temperature, but also their log$g$ value is high, so that Stark broadening is dominant in comparison with thermal Doppler broadening.

Spectral lines of zirconium are observed in stellar spectra. In particular, observations of Zr IV lines have been reported in Chayer et al. (2006), who investigated 18 sdB stars and almost always found Zr IV lines, and also in Naslim et al. (2011, 2013) and Jeffery et al. (2015).

We are preparing a large study of Stark broadening of Zr IV lines and here, as a sample of results, will be presented only Stark Full Widths at Half intensity Maximum (FWHM) for seven Zr IV lines. The complete results and the analysis of their significance for Zr IV spectral lines observed in stellar plasma will be published elsewhere (Majlinger et al., 2015). The obtained results for Stark broadening of Zr IV lines will enter in STARK-B database (http://stark-b.obspm.fr - Sahal-Bréchot et al., 2014), a node of VAMDC (Virtual Atomic and Molecular Data Centre - http://www.vamdc.eu/) since the end of 2009 (Dubernet et al., 2010, Rixon et al., 2011), so that it is also accessible via the VAMDC portal (http://portal.vamdc.org/vamdc_portal/home.sea). A link through Serbian Virtual Observatory (SerVO - http://servo.aob.rs/) is also available.

2. CALCULATION METHOD

For evaluation of Stark widths and shifts of non-hydrogenic spectral lines of ionized atoms, various theoretical approaches have been used (Griem, 1974). Both semi-classical and fully quantum-mechanical methods can be used for the evaluation of isolated line widths of multiply charged ions. Whenever there is no sufficient set of atomic data needed for a reliable semi-classical or quantum mechanical calculation, or complicated and complex calculation methods should be avoided, one can use simpler, approximate formulas. Modified semi-empirical method (MSE - Dimitrijević and Konjević, 1980) is one of such approximate approaches, whose convenience is that for calculation of electron-impact broadening parameters (widths and shifts) a considerably smaller number of atomic data, in comparison with the semi-classical method, is needed. Accuracy of MSE is usually not worse than $\pm$50%, which is in a lot of cases enough for astrophysical purposes.

3. RESULTS AND DISCUSSION

We have determined the Stark widths of seven Zr IV spectral lines (λ=1536.67 Å, λ=1598.95 Å, λ=1607.95 Å, λ=2287.38 Å, λ= 2164.36 Å,λ= 5463.85 Å, and λ= 5781.45 Å) using the MSE method, and the obtained results are shown in Table

1. The atomic energy levels of Zr IV, needed for the calculation of electron-impact full widths at half maximum (FWHM) of spectral lines are taken from Reader and Acquista (1997). The needed matrix elements are calculated using the Coulomb approximation formalism of Bates and Damgaard (1949), while the corresponding line and multiplet factors are used from Shore and Menzel (1968) in all cases when they are needed. The Stark widths are calculated for the standard plasma density of 10^{23} m^{-3}. Temperatures are within the range of 10,000 K - 500,000 K, given with unequal steps, choosen to be more frequent towards lower temperatures where the change with temperature is more pronounced. There are still no available measured Stark width data for Zr IV spectral lines, and we can compare our results only to the estimates obtained by Purić and Šćepanović (1999). Comparing the great amount of Stark width data, published by M. S. Dimitrijević, S. Sahal-Bréchot and their co-workers in numerous papers (these data are now in STARK-B database, see Sahal-Bréchot et al. 2014), Purić and Šćepanović (1999) found the correlation between Stark width and difference between ionization energy and energy of the final state.

Table 1: Stark FWHM for seven transitions of Zr IV and the electron density N_e = 10^{23} m^{-3}. Column T: Temperatures are given in 10^3 K. Column W_{MSE}: Stark widths based on our calculations using the MSE approach (Dimitrijević and Konjević 1980) given in Å; Column W_{Pur}: - Stark widths taken from Purić and Šćepanović (1999).

Zr IV, Transition, λ[Å]	T[kK]	W_{MSE}[Å]	W_{Pur}[Å]	W_{MSE}/ W_{Pur}
5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ 2287.38 Å	10	0.08435	0.06305	1.34
	20	0.05964	0.04459	1.34
	50	0.03772	0.02820	1.34
	100	0.02704	0.01994	1.36
	200	0.02154	0.01409	1.53
	300	0.01997	0.01151	1.74
	500	0.01048	0.00892	1.17
5s $^2S_{1/2}$ - 5p $^2P^o_{3/2}$ 2164.36 Å	10	0.07681	0.05645	1.36
	20	0.05431	0.03992	1.36
	50	0.03435	0.02525	1.36
	100	0.02457	0.01785	1.38
	200	0.01959	0.01262	1.55
	300	0.01811	0.01031	1.76
	500	0.01702	0.00798	2.13
5p $^2P^o_{1/2}$ - 5d $^2D_{3/2}$ 1546.17 Å	10	0.04218	0.05318	0.79
	20	0.02983	0.03760	0.79
	50	0.01887	0.02378	0.79
	100	0.01341	0.01682	0.80
	200	0.01064	0.01189	0.89
	300	0.01011	0.00971	1.04
	500	0.01005	0.00752	1.33

Zr IV, Transition, λ[Å]	T[kK]	W_{MSE}[Å]	W_{Pur}[Å]	W_{MSE}/ W_{Pur}
5p $^2P^o_{3/2}$ - 5d $^2D_{3/2}$ 1607.95 Å	10	0.04690	0.06058	0.77
	20	0.03316	0.04284	0.77
	50	0.02097	0.02709	0.77
	100	0.01488	0.01916	0.78
	200	0.01181	0.01355	0.87
	300	0.01120	0.01106	1.01
	500	0.01115	0.00857	1.30
5p $^2P^o_{3/2}$ - 5d $^2D_{5/2}$ 1598.95 Å	10	0.04631	0.05991	0.77
	20	0.03274	0.04236	0.77
	50	0.02071	0.02679	0.77
	100	0.01469	0.01916	0.77
	200	0.01166	0.01355	0.86
	300	0.01120	0.01094	1.02
	500	0.01101	0.00847	1.30
6s $^2S_{1/2}$ - 6p $^2P^o_{1/2}$ 5781.45 Å	10	1.9690	3.01090	0.65
	20	1.3920	2.12903	0.65
	50	0.9168	1.34652	0.68
	100	0.7647	0.95213	0.80
	200	0.6929	0.67326	1.03
	300	0.6597	0.54971	1.20
	500	0.6161	0.42581	1.45
6s $^2S_{1/2}$ - 6p $^2P^o_{3/2}$ 5463.85 Å	10	1.7840	2.68919	0.66
	20	1.2610	1.90155	0.66
	50	0.8283	1.20264	0.69
	100	0.6897	0.85040	0.81
	200	0.6263	0.60132	1.04
	300	0.5955	0.49098	1.21
	500	0.5573	0.38031	1.47

Using the relation derived on the basis of this correlation, they estimated Stark widths for spectral lines of a number of emitters, including Zr IV. In the second and third column of Tab. 1 there are Stark widths calculated here using MSE and calculated by Purić and Šćepanović (1999), respectively, as a function of temperature.

The dependence of the Stark width of Zr IV 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ λ= 2287.38 Å spectral line on the temperature is shown in Fig. 1, where Stark FWHM calculated here by using MSE method (Dimitrijević and Konjević 1980), is compared with the results of Purić and Šćepanović (1999) and with thermal Doppler width of the same line. Finally, using the obtained results, we investigated how Stark and Doppler width for the same spectral line change with the optical depth of the DB White Dwarf stellar atmosphere (Fig. 2). The numerical simulation is done for the optical depth corresponding to Rosseland mean opacity near the bluish green wavelenght band with the wavelenght λ= 5150 Å. To show this comparison of Stark and Doppler widths, the existing model atmosphere for DB white dwarfs is used with log g = 8 and T_{eff} =15000 K (Wickramasinghe, 1972).

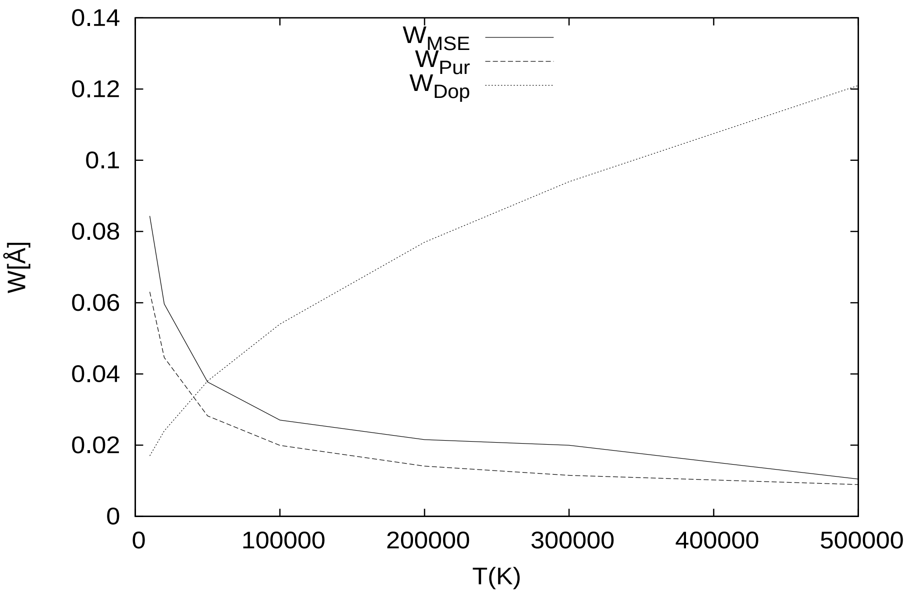

Figure 1: Comparison of Stark full widths at half maximum (FWHM) W_{MSE} - full line, calculated here by using MSE method (Dimitrijević and Konjević 1980), with the results for Stark FWHM W_{PUR} - dashed line of Purić and Šćepanović (1999) and thermal Doppler width - W_{DOP} - dotted line, for Zr IV 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ $\lambda =$ 2287.38 Å spectral line. The electron density N_e is 10^{23} m^{-3}.

The electron-impact widths obtained here by using the MSE method and those by Purić and Šćepanović (1999) are in majority in reasonable agreement taking into account that the results of Purić and Šćepanović (1999) are estimates. Their ratio increases with temperature and at 10,000 K it is 0.7-0.8 except for 5s-5p transitions, where it is 1.3-1.4. On the other hand, at 500,000 K, it is 1.7-2.1 for 5s-5p transitions and 1.3-1.5 for others. Stark broadening width decreases with temperature, and it is around 0.1 Å for T=10,000 K and around 0.6 Å for T=500,000 K, except for 6s-6p transitions where it is several times larger, reaching, at T=10,000 K 2 Å for W_{MSE} and 3 Å for W_{Pur}. It is expected, since with the increase of principal quantum number in a spectral series decreases the distance to perturbing levels and the corresponding Stark width increases. The decrease of Stark width with temperature can be also seen in Fig 1. Namely, the MSE formula for Stark widths has the inverse square root dependence at low temperature limit (Dimitrijević and Konjević 1980), while thermal Doppler broadening is purely square root dependent of temperature.

In Fig. 2 is shown the dependence of electron-impact FWHM and thermal Doppler width on logarithm of optical depth τ for standard wavelength of 5150 Å (log τ_{5150}) in the DB white dwarf atmosphere for Zr IV 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ $\lambda = 2287.38$ Å spectral line. The model atmosphere with log g = 8 and T_{eff} =15,000 K of Wickramasinghe (1972) is used. From Fig. 2 we can conclude that the electron-impact broadening has more influence on Zr IV spectrum than thermal Doppler broadening. For the investigated line, the Stark width is typically one order of magnitude larger than the Doppler one.

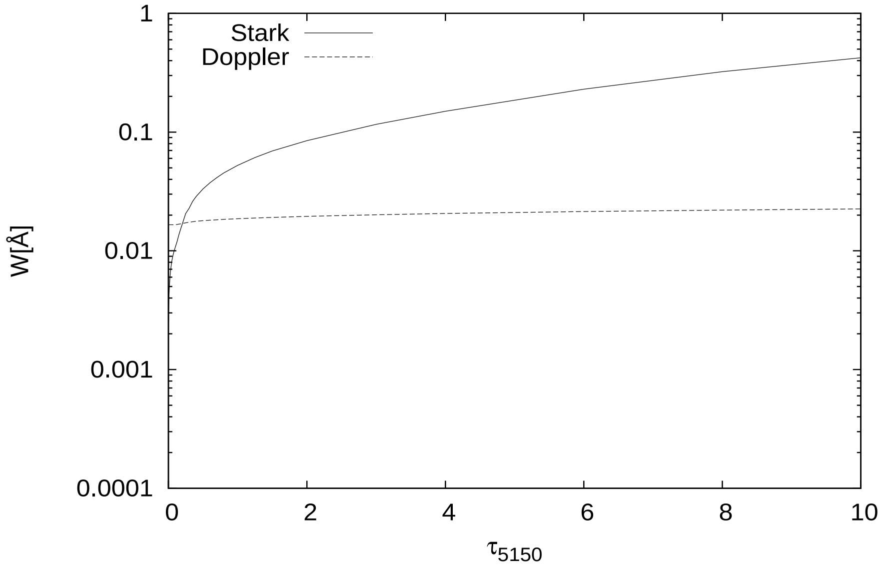

Figure 2: Dependence of electron-impact FWHM and thermal Doppler width on optical depth (log τ_{5150}) in the DB White Dwarf atmosphere for Zr IV 5s $^2S_{1/2}$ - 5p $^2P^o_{1/2}$ λ = 2287.38 Å spectral line. The model atmosphere with log g = 8 and T$_{eff}$ =15000 K of Wickramasinghe (1972) is used.

4. CONCLUSIONS

Stark FWHM for 7 Zr IV lines, needed for astrophysical plasma research, have been determined. Using the obtained results it has been demonstrated that Stark width dominates over Doppler width especially in the deeper layers of white dwarf atmosphere (difference becomes more important for larger optical depths). This conclusion concerning the importance of Stark broadening in white dwarf atmospheres is already confirmed with similar researches on spectral lines of other elements (Simić et al 2006). The difference between the Stark width and Doppler width is more resolute in white dwarf spectra than for main sequence stars, because Stark width in the impact approximation (Griem 1974) increases linearly with electron density, and it is much higher in white dwarf atmospheres. Since in Chayer et al. (2006) and Naslim et al. (2011, 2013), Zr IV lines have been used for zirconium abundance determination in several subdwarfs, we hope that Stark broadening data for Zr IV lines will be useful for further investigation of atmospheres of hot dense stars.

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