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ATOMIC DATA AND STARK BROADENING OF Nb III

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Abstract. We have calculated the electron-impact widths for 15 doubly charged Nb ion lines by using the modified semiempirical method. Here, a part of preliminary results has been presented and discussed. Using the obtained results, we considered the influence of the electron-impact mechanism on line shapes in spectra of chemically peculiar stars and white dwarfs.

1. INTRODUCTION

Atomic data for Rare Earth Elements (REE) are needed in astrophysics for example in order to solve the problems like the relative abundance of r- and s-process elements in metal-poor stars with enhanced neutron-capture abundances, but also for analysis, modelling and research of stellar atmospheres. We will determine and provide here data on broadening of Nb III spectral lines by impacts with electrons, i.e, Stark broadening data. Such data are particularly of interest for white dwarfs, but also for A-type stars and other hot stars, especially the chemically peculiar ones, since Nb is present in stellar atmospheres. Consequently, using the the modified semiempirical approach - MSE (Dimitrijević and Konjević, 1980), tested several times for complex spectra (see e.g. Popović and Dimitrijević, 1996a,b, 1997), we have determined the electron-impac (Stark) full width at half maximum intensity (FWHM) of 15 Nb III spectral lines from $4d^2$ (^3F)5s - $4d^2$ (^3F)5p transitions.

The complete results and their analysis, as well as the details of calculations will be given in Simić et al. (2014) and here only the basic information and examples of obtained results are given.

The obtained results will be used also for the research of Stark broadening and its importance for plasma conditions in atmospheres of A type stars and DB white dwarfs.

2. THEORY

In order to determine the electron-impact line widths of Nb III lines, we have used the modified semiempirical (MSE) approach (Dimitrijević and Konjević, 1980), since for this ion, there is no a sufficient number of known atomic energy levels allowing more sophysticated semiclassical perturbation (SCP) calculations (Sahal-Bréchot, 1969a,b). Namely, in comparison with SCP, a considerably smaller number of atomic data is needed for MSE method. Within the MSE approach the electron-impact (Stark) full width (FHWM) of an isolated line for an ionized emitter is given as:

$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}(\frac{2m}{\pi kT})^{1/2}\frac{\lambda^2}{\sqrt{3}} \cdot \{\sum_{\ell_i \pm 1}\sum_{L_{i'}J_{i'}} \vec{\Re}^2_{\ell_i,\ell_i \pm 1}\widetilde{g}(x_{\ell_i,\ell_i \pm 1}) +$$

$$\sum_{\ell_f \pm 1}\sum_{L_{f'}J_{f'}} \vec{\Re}^2_{\ell_f,\ell_f \pm 1}\widetilde{g}(x_{\ell_f,\ell_f \pm 1}) + (\sum_{i'}\vec{\Re}^2_{ii'})_{\Delta n \neq 0} g(x_{n_i,n_i+1}) +$$

$$(\sum_{f'}\vec{\Re}^2_{ff'})_{\Delta n \neq 0} g(x_{n_f,n_f+1})\}. \qquad (1)$$

In the above equations, the initial level is denoted with i, the final one with f, $\vec{\Re}^2_{\ell_k,\ell_{k'}}$, $k = i, f$ is the square of the matrix element, and

$$(\sum_{k'}\vec{\Re}^2_{kk'})_{\Delta n \neq 0} = (\frac{3n^*_k}{2Z})^2\frac{1}{9}(n^{*2}_k + 3\ell^2_k + 3\ell_k + 11), \qquad (2)$$

(in Coulomb approximation).

In Eq. (1)

$$x_{l_k,l_{k'}} = \frac{E}{\Delta E_{l_k,l_{k'}}}, k = i, f$$

where $E = \frac{3}{2}kT$ is the electron kinetic energy and $\Delta E_{l_k,l_{k'}} = |E_{l_k} - E_{l_{k'}}|$ is the energy difference between levels l_k and l_k ± 1 (k=i, f),

$$x_{n_k,n_k+1} \approx \frac{E}{\Delta E_{n_k,n_k+1}},$$

where for $\Delta n \neq 0$ the energy difference between energy leves with n_k and n_k+1, $\Delta E_{n_k,n_k+1}$, is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H/n^{*3}_k$. $n^*_k = [E_H Z^2/(E_{ion} - E_k)]^{1/2}$ is the effective principal quantum number, Z is the residual ionic charge, for example Z=1 for neutral atoms and E_{ion} is the appropriate spectral series limit.

With N and T are denoted electron density and temperature, respectively, while $g(x)$ (Griem, 1968) and $\widetilde{g}(x)$ (Dimitrijević and Konjević, 1980) are Gaunt factors for width, for $\Delta n \neq 0$ and $\Delta n = 0$, respectively.

The needed atomic energy levels for Nb III, have been taken from Gayazov (1998). In the Nb III spectrum configuration mixing is present. If we want to include in calculations terms which are a mixture of different configurations, we can represent them as a mixture with K_1 part of the leading configuration and K_2 of the second one, where $K_1 + K_2 = 1$, and then, we can use the expression:

$$\vec{\Re}^2_{j,j'} = K_1\vec{\Re}^2_{\alpha,\alpha'} + K_2\vec{\Re}^2_{\beta,\beta'}$$

where α, α' denote the energy level corresponding to the leading configuration, and its perturbing levels, and β, β' is the same for the second configuration (Dimitrijević and Popović, 1993).

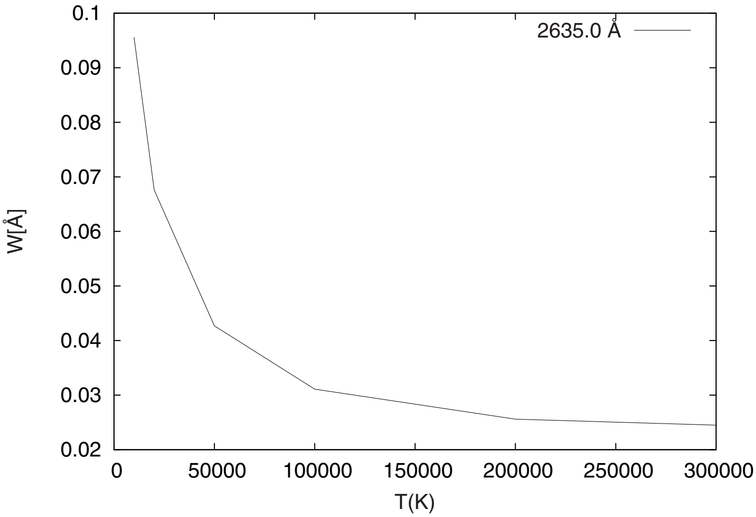

Figure 1: Stark widths for Nb III spectral line $4d^2$ (^{3}F) 5s $^4F_{5/2}$ - $4d^2$ (^{3}F) 5p $^4G^o_{5/2}$ (λ=2635.0 Å), as a function of temperature.

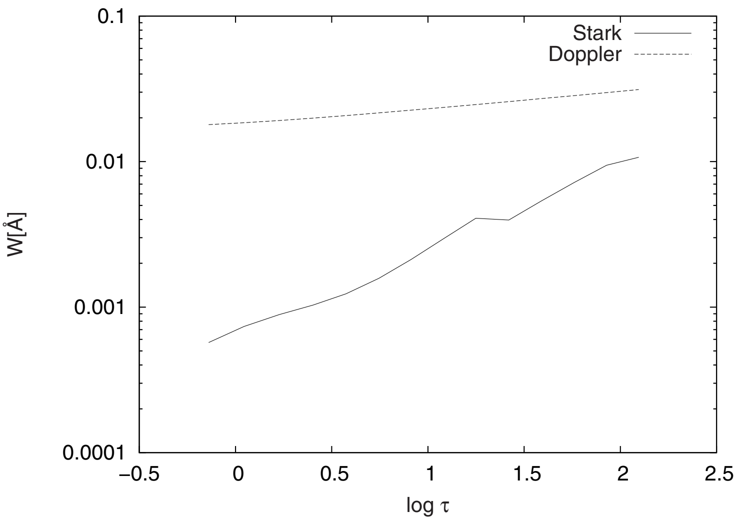

Figure 2: Thermal Doppler and Stark widths for Nb III spectral line $4d^2$ (^{3}F) 5s $^4F_{5/2}$ - $4d^2$ (^{3}F) 5p $^4G^o_{5/2}$ (λ=2635.0 Å), for an A type star atmosphere model with T_{eff} = 10,000 K and log g = 4.5, as a function of the Rosseland optical depth.

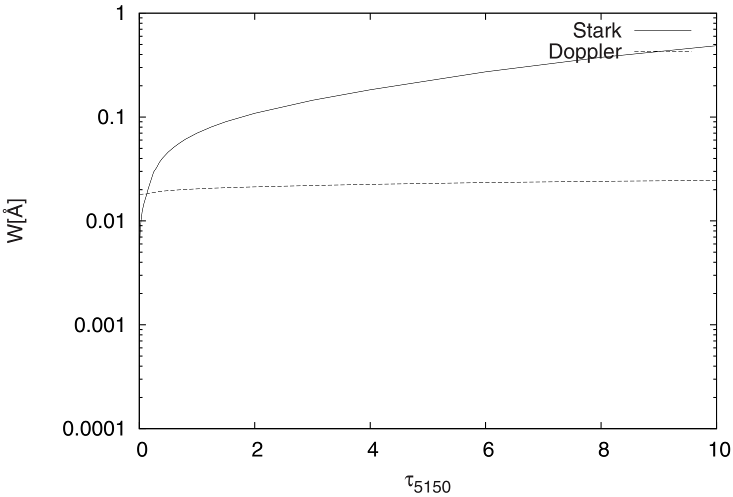

Figure 3: Thermal Doppler and Stark widths for Nb III spectral line $4d^2$ (^{3}F) 5s $^4F_{5/2}$ - $4d^2$ (^{3}F) 5p $^4G^o_{5/2}$ (λ=2635.0 Å) for a DB white dwarf atmosphere model with T_{eff} = 15,000 K and log g = 8, as a function of optical depth τ_{5150}.

3. RESULTS AND DISCUSSION

We have analyzed the Nb III spectrum and selected all spectral lines from 5s-5p transition array where the MSE method (Dimitrijević and Konjević, 1980) is applicable, and, if the configuration mixing is present, where the leading terms of initial and final energy level contribute at least 80 per cent to the corresponding term. With such constraints, 15 lines from $4d^2$ (^{3}F) 5s - $4d^2$ (^{3}G)5p have been choosen and their Stark widths determined.

In Table 1, is shown a sample of our results for Stark full width for six Nb III lines. The data are given for an electron density of 10^{17} cm^{-3} and temperatures from 10,000 up to 300,000 K. The complete results, more detailed description of calculations and the corredsponding discussion will be given in Simić et al. (2014). Here is shown in Fig. 1 the behavour of Stark width with temperature for 2635 Å line.

In Figs. 2 and 3, are compared Stark and Doppler widths for atmospheres of A-type stars and white dwarfs respectively, for Nb III line 5s $^4F_{5/2}$ - 5p $^4G^o_{5/2}$ (λ=2635.0 Å).

For A type stars, we used a model atmosphere with T_{eff} = 10,000 K and log g = 4.5 (Kuruczs, 1979), and for DB white dwarfs a model with T_{eff} = 15,000 K and log g = 8 (Wickramasinghe, 1972). We note that for the DB white dwarfs, the prechosen optical depth points at the standard wavelength λ_s=5150 Å(τ_{5150}) are used in (Wickramasinghe, 1972), as well as in our Fig. 3, because of this. This is different from the A type star model (Kuruczs, 1979), where the Rosseland optical depth scale (τ_{Ross}) has been taken, as well as for our Fig. 2. From Figs. 2 and 3 one can see that in the considered DB white dwarf atmosphere thermal Doppler broadening has much less importance in comparison with the Stark broadening mechanism than in A-type stellar atmospheres.

We can see that especially for white dwarf atmosphere analysis, the obtained Nb III Stark broadening data will be of interest.

Table 1: This table presents Nb III electron-impact broadening parameters (full width at half maximum W) for $4d^2$ (^3F) 5s - $4d^2$ (^3F) 5p transitions obtained by the modified semiempirical method (Dimitrijević and Konjević, 1980) for a perturber density of 10^{17} cm^{-3} and temperatures from 10,000 up to 300,000 K.This a sample of six lines and the complete results will be published in Simić et al. (2014).

Transition	T(K)	W(Å)	Transition	T(K)	W(Å)
	10000.	0.929-01		10000.	0.858-01
	20000.	0.657-01		20000.	0.607-01
$^4F_{3/2}$ - $^4G^o_{5/2}$	50000.	0.415-01	$^4F_{9/2}$ - $^4F^o_{7/2}$	50000.	0.384-01
2599.7 Å	100000.	0.302-01	2469.5 Å	100000.	0.278-01
	200000.	0.249-01		200000.	0.228-01
	300000.	0.238-01		300000.	0.219-01
	10000.	0.736-01		10000.	0.823-01
	20000.	0.521-01		20000.	0.582-01
$^4F_{3/2}$ - $^4D^o_{1/2}$	50000.	0.329-01	$^4F_{9/2}$ - $^4F^o_{9/2}$	50000.	0.368-01
2274.6 Å	100000.	0.238-01	2414.7 Å	100000.	0.267-01
	200000.	0.195-01		200000.	0.218-01
	300000.	0.188-01		300000.	0.210-01
	10000.	0.988-01		10000.	0.956-01
	20000.	0.698-01		20000.	0.676-01
$^4F_{9/2}$ - $^4G^o_{7/2}$	50000.	0.442-01	$^4F_{5/2}$ - $^4G^o_{5/2}$	50000.	0.427-01
2657.3 Å	100000.	0.321-01	2635.0 Å	100000.	0.311-01
	200000.	0.264-01		200000.	0.256-01
	300000.	0.253-01		300000.	0.245-01

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