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Stark broadening data for spectral lines of rare-earth elements: Nb III ☆

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Abstract

The electron-impact widths for 15 doubly charged Nb ion lines have been theoretically determined by using the modified semiempirical method. 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.

Keywords: Rare-earths; Line profiles; Atomic data

1. Introduction

Spectral lines of rare earth elements (REE) are present in stellar spectra, especially in spectra of chemically peculiar (CP) ones and white dwarfs. Consequently, data on the Stark broadening of REE spectral lines are of interest not only for laboratory but also for astrophysical plasma research as e.g. for REE abundance determination and opacity calculations. The lines of Nb II are observed in spectra of cool Ap star γ Equulei in the spectral region $\lambda\lambda$ 3086–3807 (Adelman et al., 1979). Fuhrmann (1989) investigated eleven high resolution IUE spectra of the CP star H465 and reported presence of spectral lines for singly ionized niobium among the other REE ions, which are quite strong in the optical spectra.

Atomic data for REE are needed in order to solve the astrophysical problems such as the relative abundance of r- and s-process elements in metal-poor stars with enhanced neutron-capture abundances. Slow neutron-capture process, the s-process occurs when the star is in the ”asymptotic giant branch” phase of its life. Nilsson et al. (2010) derived accurate transition probabilities for astrophysically interesting spectral lines of Nb II and Nb III and determined the niobium abundance in the Sun and metal-poor stars rich in neutron-capture elements. Also, Nilsson et al. (2010) derived solar photospheric niobium abundance, obtaining the result log $\epsilon_{Sun} = 1.44 \pm 0.06$, in agreement with the meteoritic value.

Due to very complex spectra of REE it is not always possible to apply the same method to calculate the Stark broadening data (see, (Popović and Dimitrijević, 1998)). Also, there is many cases with incomplete number of atomic data, when an estimate of Stark broadening parameters on the basis of regularities and systematic trends can be possible (Dimitrijević and Popović, 1989).

In order to provide a complete set of Stark broadening data of astrophysical interest, Popović and Dimitrijević (1998) started and Popović et al. (1999) continued a project to theoretically determine such data for a number of spectral lines of REE.

Gayazov et al. (1998) improved and extended the previous analyses of the Nb III spectrum on the basis of new, high resolution, observations and modern technique of spectrum identification. The spectrum of doubly charged Nb ion is recorded in the region 900–2512 Å with the aid

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of a 6.65 m vacuum ultraviolet normal incidence spectrograph. As a result of this work, the list of identified Nb III transitions contains 908 lines, including about 300 previously classified lines. Gayazov et al. (1998) noted that LS-coupling is a quite good approximation in the studied configurations for niobium. We note however, that there is many energy levels of Nb III with mixing of configurations.

Here, we have applied the modified semiempirical approach – MSE (Dimitrijević and Konjević, 1980) whose applicability for complex spectra has been tested several times (see e.g. (Popović and Dimitrijević, 1996a; Popović and Dimitrijević, 1996b; Popović and Dimitrijević, 1997)), for the determination of electron-impac (Stark) full width at half maximum intensity (FWHM) of 15 Nb III spectral lines from 4d^2 (^{3}F)5s–4d^2 (^{3}F)5p transitions. The obtained results will be used to investigate the importance of Stark broadening for plasma conditions in atmospheres of A type stars and DB white dwarfs.

2. Theory

For the determination of electron-impact line width Nb III lines, the modified semiempirical (MSE) approach (Dimitrijević and Konjević, 1980) has been used. It is suitable, since in comparison with the semiclassical perturbation approach (Sahal-Bréchot, 1969a; Sahal-Bréchot, 1969b), it needs a considerably smaller number of atomic data, and, for Nb III, there is no a sufficient number of known atomic energy levels allowing more sophysticated semiclassical perturbation calculations. Within the MSE method, the electron-impact (Stark) full width (FHWM) of an isolated ion line, is given for an ionized emitter as:

$$w_{MSE} = N\frac{4\pi}{3c}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\lambda^2}{\sqrt{3}}\cdot\Bigg\{\sum_{\ell_i\pm1}\sum_{L_{i'}J_{i'}}\vec{\Re}^2_{\ell_i,\ell_i\pm1}\widetilde{g}(x_{\ell_i,\ell_i\pm1}) + \sum_{\ell_f\pm1}\sum_{L_{f'}J_{f'}}\vec{\Re}^2_{\ell_f,\ell_f\pm1}\widetilde{g}(x_{\ell_f,\ell_f\pm1}) + \left(\sum_{i'}\vec{\Re}^2_{ii'}\right)_{\Delta n\neq0} g(x_{n_i,n_i+1}) + \left(\sum_{f'}\vec{\Re}^2_{ff'}\right)_{\Delta n\neq0} g(x_{n_f,n_f+1})\Bigg\}, \quad (1)$$

where 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

$$\left(\sum_{k'}\vec{\Re}^2_{kk'}\right)_{\Delta n\neq0} = \left(\frac{3n_k^*}{2Z}\right)^2\frac{1}{9}(n_k^{*2} + 3\ell_k^2 + 3\ell_k + 11), \quad (2)$$

(in Coulomb approximation).

In Eq. (1)

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

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 $l_k \pm 1$ $(k = i, f)$,

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

where for $\Delta n \neq 0$ the energy difference between energy levels with n_k and n_k+1, $\Delta E_{n_k,n_k+1}$, is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2E_H/n_k^{*3}$. $n_k^* = [E_HZ^2/(E_{ion} - E_k)]^{1/2}$ 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.

In Eqs. (1) and (2) N and T are electron density and temperature, respectively, while with $g(x)$ (Griem, 1968) and $\widetilde{g}(x)$ (Dimitrijević and Konjević, 1980) are denoted Gaunt factors for width, for $\Delta n \neq 0$ and $\Delta n = 0$, respectively.

Atomic energy levels needed for calculation of Nb III Stark line widths have been taken from Gayazov et al. (1998). In the Nb III spectrum configuration mixing is present so that exist terms which are a mixture of different configurations. If we can not neglect the contribution of other configurations, for any term represented as a mixture with K_1 part of the leading configuration and K_2 of the second one, where $K_1 + K_2 = 1$, 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).

3. Results and discussion

Calculations of Stark widths for doubly charged niobium ion lines have been carried out for fifteen 4d^2 (^{3}F)5s–4d^2 (^{3}F)5p transitions. We have selected all spectral lines from Nb III 5s-5p transition array where it is possible to apply MSE approach (Dimitrijević and Konjević, 1980), and where the contributions of leading term of initial and final energy level are at least 80 per cent.

In Table 1, our results for Stark full width for 4d^2 (^{3}F)5s–4d^2 (^{3}F)5p transitions of doubly charged niobium ion spectral lines, are shown. The data are given for an electron density of 10^{17} cm^{-3} and temperatures from 10,000 up to 300,000 K. Here, we draw attention to the 2415.2 Å spectral line of Nb III for transitions 5s $^4F_{7/2}$–5p $^4F^o_{7/2}$ with a relative intensity of 1000 (Gayazov et al., 1998).

In order to show how much is important to take into account the Stark broadening for the modelling and analysis of A type star and DB white dwarf atmospheres, we compared thermal Doppler and Stark broadening in the both cases.

For A type stars, we used a model atmosphere with $T_{eff} = 10{,}000$ K and $\log g = 4.5$ (Kuruczs, 1979). In Fig. 1, we compared thermal Doppler and Stark widths for Nb III spectral line 5s $^4F_{7/2}$–5p $^4F^o_{7/2}$ ($\lambda = 2415.2$ Å).