NLTE CALCULATION FOR O II

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ABSTRACT. The Kurucz's atmospheric models and a modified version of the MULTI code are applied in a NLTE investigation of the O II spectrum. It is shown that previously performed analyses based on the use of lightly line-blanketed Gold models give results that are in variance with those based on the use of the more heavily blanketed Kurucz's models.

One result of our calculations is a number of useful relationships between the NLTE oxygen abundance, line equivalent width, and stellar atmospheric parameters.

Key words:Stars: abundances – Stars: early type– NLTE -analysis

1. Introduction

Oxygen, one of the most abundant elements, is preferentially formed during explosive nucleosynthesis in Type II supernovae. Despite the participation of the oxygen nuclei in the CNO cycle of hydrogen burning in massive stars, the oxygen abundance is not expected to be significantly altered during the standard evolution of the star from the main sequence to red giant region, much less while the star still resides on the main sequence. Thus, surface oxygen abundances in main sequence B stars should reflect the initial oxygen content in the interstellar medium from which the stars are formed. an investigation of oxygen abundance variations among B stars can accordingly much say about the efficiency of Type II supernovae and possible inhomogeneities within the progenitor material of the B stars.

In the present work we report results from NLTE O II calculations which were performed using a modified version of the MULTI code. The MULTI code has not been used in previously published NLTE determinations of oxygen abundances (e.g. Becker & Butler 1988a). We consider our approach a more realistic one relative to the Becker & Butler analysis as it is based on the use of Kurucz model atmospheres while the Becker & Butler calculations were based upon less line-blanketed models which we feel do not present an adequate description of the atmospheres of early-type stars.

2. NLTE calculations

Simultaneous solution of the radiative transfer and statistical equilibrium equations have been realized using the MULTI-code (Carlsson, 1986) in the approximation of complete frequency redistribution for all lines. The initial version of this code was modified with the aim to apply it in the analysis of early-type stars. In particular,

1) we have included in the code opacity sources from the ATLAS9 program (Kurucz, 1992). This enables a much more accurate calculation of the continuum opacity and intensity distribution in the UV region which is extremely important in the correct determination of the radiative rates of $b-f$ transitions;

2) we have changed the code to calculate the combined profile of blended lines taking into account stellar rotation and instrumental profiles.

In addition to these modifications, we for the first time have applied to the analysis of O II lines in the spectra of hot stars the well-known blanketed atmosphere models of Kurucz (1992).

2.1. Parameters of the oxygen atom

We employed a model oxygen atom consisting of 141 levels: 3 levels in O I, 132 levels in O II with $L \leq 5$ and $n \leq 8$, 5 levels in O III, and the ground state of O IV. The detailed structure of the multiplets was ignored and each LS multiplet was considered as a single term.

Within the described system of oxygen atom levels we considered the radiative transitions between the first 49 levels of O II and the ground level of O III. These energy levels were selected from the compilation of Hirata & Horaguchi (1994). Transitions between the remaining levels were not taken into account and those levels were used only in the equations of population conservation.

Only transitions having $\lambda < 100\,000\,\AA$ were considered. After numerous test calculations, 86 $b-b$ transitions were included in the linearization procedure. These transitions describe quite well the formation of the lines of interest. Another 170 transitions were treated as having fixed radiative rates.

Photoionization cross-sections were mainly taken from the Opacity Project (Yan et al., 1987) keeping account within the calculations of the detailed structure of their frequency dependence, including resonances.

Oscillator strengths were selected from the extensive compilation of Hirata & Horaguchi (1994), from the survey of lines which are formed as transitions from the ground level by Verner et al., (1994) and from CDROM 23 of Kurucz (1994). Some information was also obtained through the Opacity Project. As we ignored the multiplet structure of all levels, the oscillator strength for each averaged transition was calculated as $f = \frac{\sum g_i f_i}{\sum g_i}$.

After the combined solution of the radiative transfer and statistical equilibrium equations, the average level populations were redistributed proportional to the statistical weights of the corresponding sublevels to regain the detailed multiplet structure, and finally the lines of the interest were investigated.

Stark parameters are a very important part of the analysis as their influence on the resulting oxygen abundance as derived from O II lines is rather significant. To calculate the Stark parameters for the considered transitions we used the semiempirical formula provided by Dimitrijević (1997) for the full width at the half maximum (FWHM):

$$\begin{aligned} W(\mathring{A}\,) &= 2.2151 \cdot 10^{-8} \frac{\lambda^2(cm) N(cm^{-3})}{T^{1/2}(K)} * \\ &\left(0.9 - \frac{1.1}{Z}\right) \sum_{k=i,j} \left(\frac{3n_k^*}{2Z}\right)^2 * \\ &\left(2n_k^{*2} - l_k^2 - l_k - 1\right) \end{aligned} \tag{1}$$

Here n^* is an effective principal quantum number and l is an angular momentum quantum number. Calculations using this formula were performed for T=20 000K.

Collisional ionization interactions were described using Seaton's formula (Seaton, 1962):

$$C_{ik} = 1.55 \cdot 10^{13} \frac{\alpha(\nu_0) \overline{g} N_e e^{-u_0}}{\sqrt{T_e} u_0} \tag{2}$$

where $\alpha(\nu_0)$ is the threshold value of the cross-section, $u_0 = \frac{E_0}{kT_e}$, E_0 is the energy of ionization, and N_e and T_e are the electron density and temperature respectively. For the Gaunt factor we adopted a value of 0.3. For all allowed $b-b$ transitions we used the van Regemorter (1962) formula:

$$\begin{aligned} C_{ij} &= 5.465 \cdot 10^{-11} N_e \sqrt{T_e} \cdot 14.5 f_{ij} \left(\frac{I_H}{E_0}\right)^2 * \\ &u_0 e^{-u_0} \max\left[\overline{g}; 0.276 e^{u_0} E_1\left(u_0\right)\right] \end{aligned} \tag{3}$$

where I_H is the hydrogen ionization potential and $E_1\,(u_0)$ is the first-order integral exponential function. Collisional rates for forbidden transitions were calculated with the help of a semiempirical formula (Allen, 1973), with collisional force of 1:

$$C_{ij} = 8.63 \cdot 10^{-6} \frac{N_e e^{-u_0}}{g_i \sqrt{T_e}} \tag{4}$$

3. General results of the calculation

Applying the above prescription we made an attempt to find relationships between the oxygen abundance and oxygen line equivalent width for a range of atmosphere parameters ($T_{\rm eff}$ ranging from 20 000 K to 33 000 K; V_t from 1 $km\ s^{-1}$ to 8 $km\ s^{-1}$ and oxygen abundance (O/H) from 8.37 to 8.87). Approximations were found for three different gravity values: 3.50, 3.75 and 4.00. We found that the NLTE oxygen abundance can be expressed by the following formula:

$$\begin{aligned} (O/H)_{NLTE} &= 10^{\left(a\cdot T_{\rm eff} + b\cdot V_t + c\cdot \log(W) + d\cdot T_{\rm eff}^2\right)} * \\ &10^{\left(e\cdot T_{\rm eff}^4 + f\cdot T_{\rm eff}^5 + g\cdot(\log(W))^2\right)} \end{aligned} \tag{5}$$

Coefficients (for selected O II lines) to be used in this formula are listed in Table **??**- **??** for the different log g values. For this fitting formula $\sigma = 0.02$ with a maximum deviation of 0.1 dex. We hope that this relationship will be of use in the determination of oxygen abundances in hot main sequence stars.

4. Comparison with previous studies

For illustration, in Fig. **??** - **??** we present individual dependencies between a) line equivalent width and effective temperature for a selection of O II lines which were investigated by Becker & Butler 1988b calculated with (O/H)=8.88 and $\log g$ = 4.0 and b) equivalent width and relative oxygen abundance (V_t=5 $km\ s^{-1}$, $\log g$ =4.0 and $T_{\rm eff}$=30 000 K).

Note that in the figures we have reproduced only the Becker & Butler (1988b) NLTE results. As one can see from these figures our NLTE equivalent widths are systematically stronger than those derived by Becker & Butler. For the majority of the investigated lines Becker & Butler obtained NLTE equivalent widths which are practically the same as those derived by us in the LTE approximation. The Becker & Butler (1988a, 1988b) calculations were performed using the grid of Gold (1984) models which only take into account the blanketing from the 104 strongest lines present in the spectra of B stars. In our study, the more heavily blanketed Kurucz models were used. We believe that the main source of the disparity between these NLTE results originates in the grids of atmospheric models used

Table 1: Coefficients for $\log g = 4.0$

λ	a	b	c	d	e	f	g
4595.96	1.5124159E-04	-2.0471793E-03	1.1170454E-02	-6.9585345E-09	5.6306715E-18	-8.3406351E-23	2.5195905E-02
4609.43	1.5550496E-04	-1.9760641E-03	3.7945134E-02	-7.2792605E-09	6.0706978E-18	-9.1441341E-23	1.7967415E-02
4610.20	1.5342524E-04	-6.4951778E-04	5.4851509E-02	-7.0222524E-09	5.8144563E-18	-8.7656958E-23	5.2823667E-03
4638.85	1.5098142E-04	-2.9185301E-03	5.3815554E-03	-6.9548807E-09	5.6546257E-18	-8.3610841E-23	3.0510199E-02
4641.81	1.5556961E-04	-4.2725404E-03	-2.0024990E-02	-7.3153636E-09	6.1042202E-18	-9.1532692E-23	4.1677337E-02
4649.14	1.5747199E-04	-5.1880087E-03	-2.8205318E-02	-7.5325189E-09	6.4400702E-18	-9.7818988E-23	4.6517209E-02
4650.84	1.5099143E-04	-2.9357199E-03	4.9863263E-03	-6.9583613E-09	5.6634497E-18	-8.3799094E-23	3.0643451E-02
4661.63	1.5228854E-04	-3.3137111E-03	-3.1963094E-03	-7.0562897E-09	5.7812318E-18	-8.5851170E-23	3.4133706E-02
4673.74	1.4803582E-04	-1.2051937E-03	4.4609172E-02	-6.7489229E-09	5.5337076E-18	-8.2534395E-23	1.1919067E-02
4676.24	1.5139794E-04	-3.0697621E-03	1.7360954E-03	-6.9924989E-09	5.7116551E-18	-8.4694643E-23	3.1920778E-02
4701.18	1.5169998E-04	-8.2484372E-04	5.0335866E-02	-6.9317828E-09	5.7352080E-18	-8.7010008E-23	7.8638346E-03
4701.71	1.5261058E-04	-2.6835721E-04	5.2427504E-02	-6.8918749E-09	5.7108517E-18	-8.7095172E-23	3.1452259E-03
4703.16	1.5283858E-04	-1.1437849E-03	4.8370093E-02	-7.0431963E-09	5.8077093E-18	-8.7432427E-23	1.0043059E-02
4705.35	1.5583200E-04	-2.9512437E-03	1.3518314E-02	-7.3146649E-09	6.0608582E-18	-9.0682382E-23	2.8147661E-02

Table 2: Coefficients for $\log g = 3.75$

λ	a	b	c	d	e	f	g
4595.96	1.5818248E-04	-2.3497411E-03	8.3003630E-03	-7.5308156E-09	6.4044870E-18	-9.6876532E-23	2.8641347E-02
4609.43	1.6206867E-04	-2.1993521E-03	4.0001418E-02	-7.8348275E-09	6.8434770E-18	-1.0496580E-22	1.9773060E-02
4610.20	1.6145329E-04	-7.1977819E-04	5.8161035E-02	-7.6947409E-09	6.8336005E-18	-1.0659798E-22	4.9297307E-03
4638.85	1.5762685E-04	-3.4791378E-03	9.8773155E-03	-7.5576263E-09	6.5305826E-18	-9.9256489E-23	3.3043315E-02
4641.81	1.6260848E-04	-4.8742939E-03	-2.1495756E-02	-7.9535248E-09	7.0787165E-18	-1.0952849E-22	4.5668031E-02
4649.14	1.6528388E-04	-5.7827268E-03	-3.8418733E-02	-8.2057405E-09	7.4888534E-18	-1.1759610E-22	5.2269174E-02
4650.84	1.5768924E-04	-3.4996126E-03	9.3298543E-03	-7.5656412E-09	6.5476069E-18	-9.9616927E-23	3.3237900E-02
4661.63	1.5916635E-04	-3.8998935E-03	-7.5546154E-04	-7.6788990E-09	6.6992830E-18	-1.0243329E-22	3.7288605E-02
4673.74	1.5317344E-04	-1.4847151E-03	5.3207010E-02	-7.2146370E-09	6.2153895E-18	-9.4618969E-23	1.1129314E-02
4676.24	1.5825738E-04	-3.6460966E-03	5.1309199E-03	-7.6127789E-09	6.6202295E-18	-1.0103721E-22	3.4819245E-02
4701.18	1.6217063E-04	-9.9795688E-04	5.5854237E-02	-7.8090002E-09	7.0897737E-18	-1.1299280E-22	7.8873099E-03
4701.71	1.6582553E-04	-3.1353119E-04	5.5320693E-02	-7.9823693E-09	7.4359338E-18	-1.2066954E-22	2.3231178E-03
4703.16	1.5868826E-04	-1.3369163E-03	5.0029739E-02	-7.5227508E-09	6.4489943E-18	-9.8501747E-23	1.1559815E-02
4705.35	1.6194701E-04	-3.2342595E-03	1.0843579E-02	-7.8196774E-09	6.7273954E-18	-1.0192404E-22	3.1383322E-02

Table 3: Coefficients for $\log g = 3.5$

λ	a	b	c	d	e	f	g
4595.96	1.6079796E-04	-2.5305435E-03	1.6841984E-02	-7.8929755E-09	7.1144087E-18	-1.1062902E-22	2.6620385E-02
4609.43	1.6496742E-04	-2.4034305E-03	4.1862426E-02	-8.1890307E-09	7.5067666E-18	-1.1731028E-22	1.9926116E-02
4610.20	1.5921632E-04	-8.2052104E-04	5.8927117E-02	-7.5960925E-09	6.7073715E-18	-1.0275765E-22	5.6171124E-03
4638.85	1.5795731E-04	-3.7836232E-03	1.7160895E-02	-7.7252475E-09	6.8833710E-18	-1.0536840E-22	3.2206704E-02
4641.81	1.6505913E-04	-5.4637484E-03	-2.3209422E-02	-8.2717780E-09	7.6452575E-18	-1.1975818E-22	4.8391266E-02
4649.14	1.6932802E-04	-6.5899926E-03	-4.8219516E-02	-8.6316391E-09	8.2155537E-18	-1.3102738E-22	5.7763210E-02
4650.84	1.5803201E-04	-3.8061369E-03	1.6705296E-02	-7.7353770E-09	6.9057767E-18	-1.0585360E-22	3.2390344E-02
4661.63	1.6001377E-04	-4.2796142E-03	4.9433570E-03	-7.8876596E-09	7.1146639E-18	-1.0977545E-22	3.7236508E-02
4673.74	1.5195166E-04	-1.5761129E-03	5.4466399E-02	-7.2096549E-09	6.2760012E-18	-9.5001266E-23	1.1237115E-02
4676.24	1.5871367E-04	-3.9762727E-03	1.2465191E-02	-7.7945504E-09	7.0006491E-18	-1.0774082E-22	3.4108289E-02
4701.18	1.6058249E-04	-1.0406804E-03	6.3991701E-02	-7.8080825E-09	7.2441869E-18	-1.1638921E-22	4.6312505E-03
4701.71	1.6119949E-04	-3.1750974E-04	5.5109248E-02	-7.6997140E-09	7.1124958E-18	-1.1455931E-22	2.2297030E-03
4703.16	1.6130156E-04	-1.4516562E-03	5.4553511E-02	-7.8557148E-09	7.1009259E-18	-1.1113663E-22	1.0287603E-02
4705.35	1.6823938E-04	-3.5500940E-03	8.2575492E-03	-8.4236977E-09	7.7444909E-18	-1.2102193E-22	3.3036626E-02

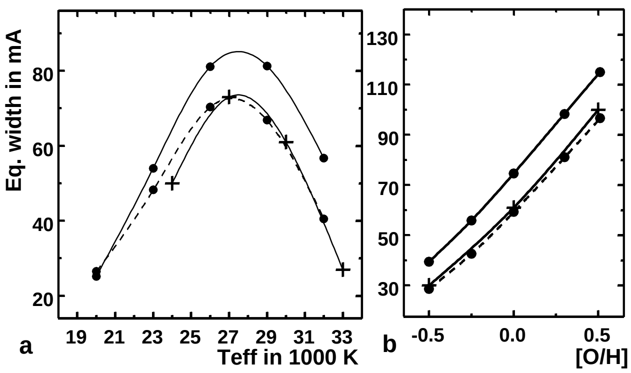

Figure 1: Equivalent width of 4078.84 Å line versus $T_{\rm eff}$ -**a** and[O/H] -**b** for NLTE (solid line) and LTE (dashed line). Our results are indicated by filled circles and those of Becker & Butler (1988b) by crosses.

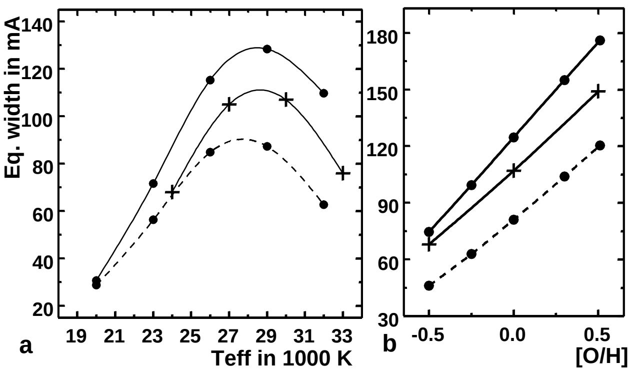

Figure 2: Same as Fig. **??**, but for 4185.45 Å .

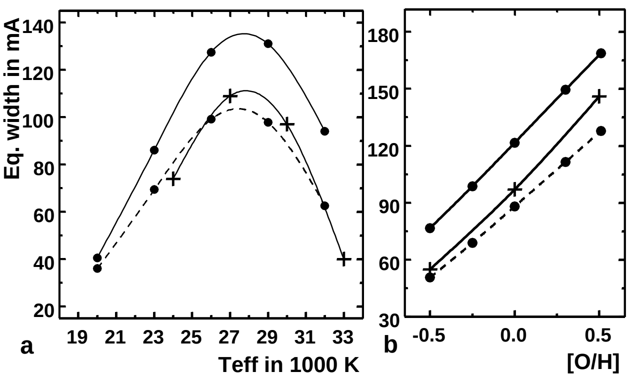

Figure 3: Same as Fig. **??**, but for 4638.86 Å .

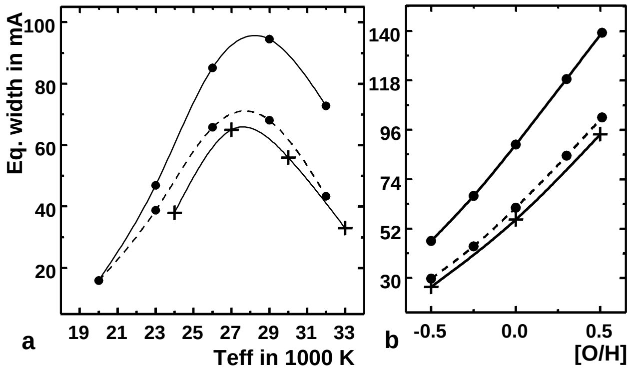

Figure 4: Same as Fig. **??**, but for 4906.83 Å .

in the respective analyses. In fact, it was first noted by Cunha & Lambert (1994) that in NLTE determinations of elemental abundances in hot stars that the more heavily blanketed models should produce a more realistic result. Later, Korotin et al. (1999) discussed this problem having presented direct NLTE calculations of the nitrogen abundance in γ *Peg* based on Kurucz models.

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