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Model atmosphere program _STAR

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A computer program for calculation of blanketed LTE model atmospheres for stars of spectral classes O–K is presented. Allowance for the opacity in lines is made by the method of opacity sampling, and about 500000 spectral lines are used for the calculation. For stars of spectral class *F* and later convection and molecular absorption in 27 main bands are taken into account.

The main advantage of the program, as compared to the complex ATLAS9 widely used today, is the possibility of independent changing of separate chemical element abundances and construction of model atmospheres of chemically peculiar stars.

The program is tested by comparing model atmospheres of stars, calculated by us, with the models of Kurucz and Fuhrmann.

Key words: stars: atmospheres – methods: numerical

1. Introduction

One of the ways of obtaining information about physical characteristics of stars is comparing the observed energy distributions in their spectra with those obtained from models. For this purpose, we need to construct a self-consistent model adequate for a star atmosphere where the radiation coming to us is formed.

By now, many programs for solving this problem are available. Probably, the most usable are the programs of the *ATLAS* family created by Kurucz, and the already computed with their help model grids for different sets of physical parameters.

Here we presented a development of one of the versions of these codes (*ATLAS*5).

The majority of the existing programs take account of the opacity in lines by method of Opacity Pretabulated Distribution Functions (OPDF), where we deal with opacity tables for every frequency interval, calculated once for all.

The advantage of such an approach is that having once spent much computing time for the construction of OPDF tables and calculated them for definite step of changing of the parameters, one does not need to return to this procedure again. This is important since it is the opacity calculation that takes a considerable amount of computation time, and such a method makes it possible to take into account $\sim 10^7$ of spectral lines. However, it is exactly the weak point in the method: we cannot calculate a model atmosphere for the chemical composition, which differs from that presented in the existing grid of *OPDF* tables. But such a necessity does exist. In particular, for spectral study of chemically peculiar stars one must be able to calculate model atmospheres having any chemical composition. Thus, the complex *_STAR* (STellar Atmosphere Researching code) presented in this paper solves exactly this problem, allowing calculation of blanketed LTE model atmosphere having any, even the most unexpected chemical composition, with consideration of about 500000 basic spectral lines.

This problem can be solved with the help of the complex *ATLAS* 12, and the program presented in this paper is an analog of the latter. However, the *ATLAS* 12 package does not have free distribution and is not accessible in the form of primary files, so creation of a complex having analogous features has an important applied significance and makes it possible to conduct independent modeling of star atmospheres.

Calculation of models is possible for stars of spectral class O–K. For stars of class *F* and later, the convection and basic molecular absorption bands are considered.

2. Model atmosphere program *_STAR*

The offered program calculates a stationary plane-parallel blanketed LTE model of the star atmosphere. *_STAR* is the development of the complex

ATLAS5 created by Kurucz (it is described in detail in the paper of Kurucz (1970)) and is realized in the FORTRAN programming language (NDP-FORTRAN version).

At the first calculation stage a grey model atmosphere is being constructed or a model obtained by means of our program or some other programs may be used. The building of a grey model implies solution of the equation of hydrostatic equilibrium for gray temperature distribution, i.e. such one, as it would be if absorption coefficient was independent of the frequency. This approximation is far from reality but is described analytically. In particular, for convective models the temperature distribution differs from that of the initial grey model so much that it was more efficient to take as the first approximation the Kurucz's (1994) model atmosphere for corresponding parameters.

As a rule, 70–100 points by depth are given in the model, which are equally distributed on a logarithmic scale of Rosseland optical depths (usually a range of $10^{-6} - 100\tau_{ross}$ is used). As a result, for each point of this grid of depth, we obtain temperature, gas pressure and concentration of particles. Using these data in the context of LTE, by assigning relative abundances we can calculate the concentration of any element at any ionization stage. So we can do the same for opacity at any frequency.

A stellar model atmosphere must satisfy the energy balance equation, i.e. each elementary volume of atmosphere must lose as much energy as it gets. In other words, the full energy flux (radial and convective) at any depth of the atmosphere must be equal to the outgoing radial energy flux $4\pi H_0 = \sigma T_{eff}^4$, and its derivative must be equal to zero. Naturally, the initial model does not satisfy the energy balance condition, therefore the final model is obtained by iterations. At each iteration, for each point of depth grid the difference between the calculated integral flux and the value $4\pi H_0$ is found, and using this difference, correction to the actual temperature is obtained. The standard methods of temperature correction (Kurucz 1970) are used in the program. The number of iterations is predetermined before the beginning of calculations. The model is considered reasonable, if the integral flux determination error does not exceed 1% for models with radiative envelope, and 10–15% for models with convection, which converge essentially worse and slower. Usually, to get a reasonable model, we need from 10 to several tens, and even hundreds (for convective models) of iterations.

To calculate the radiation flux magnitude during each iteration, it is necessary to solve the radiation transfer equation for a large number of frequencies:

$$\cos\theta \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu,$$

where I_ν is radiation flux intensity, S_ν is source function, defined as:

$$S_\nu = \frac{\kappa_\nu}{\kappa_\nu + \sigma_\nu} B_\nu + \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu} I_\nu.$$

Here, σ_ν is dispersion coefficient, B_ν is Plank function, κ_ν is true absorption coefficient.

As we have already noted, to build an adequate model of the stellar atmosphere, we need to consider opacity not only in the continuum, but also in a large number of spectral lines. Since it seems impossible to precisely consider the influence of each line under study, the following method was chosen. The entire spectral range $3 \times 10^{13} - 3 \times 10^{20}\mathrm{s}^{-1}$ considered for the given model, is divided into a large number (up to 40000) of bands, equidistributed on the frequency logarithmic scale. For the central frequency of each band, at each given optical depth, the opacity is calculated accurately both in the continuum and in nearby spectral lines. Then, we believe that the opacity for entire considered narrow band of frequencies is the same as at the central frequency of this band. In general, it is not so, but when fragmenting the whole spectral interval into sufficiently large number of narrow bands, it is possible to accurately restore both the radiation integrated flux and its spectral distribution. During calculations the lines of neutral atoms and the first five ions of elements with atomic numbers $Z \leq 30$ are considered, and for other elements 3 ionization stages are taken into account. To build blanketed model atmospheres, we used about 500000 lines taken from Kurucz (1994). This number makes it possible, at a reasonable machine time, to allow very accurately the opacity in all spectral ranges. Because of the large number of lines, a screening procedure was applied to those which do not contribute to the opacity at the given frequency. Lines whose center is away from the given frequency by more than 35Å, and lines giving a negligible contribution to the opacity were screened.

For stars with different temperatures the main contribution to the total absorption coefficient at each frequency will be given by different opacity sources, and the ways of energy transfer in the atmosphere will be different too. Thus, in the atmospheres of stars of class A and earlier the radiative transfer is predominant. For stars of class F and later ($T_{eff} < 8000K$) we must take into account the energy transfer by convective flows, and influence of molecular absorption bands, playing an important role for stars of class later than G.

The calculation of molecular absorption coefficient was made by the method of "blurred lines" which was applied for vibronic bands of biatomic molecules in the visible region of the spectrum (Pavlenko, Yakovina 1994). The essence of calculation consists in computation of the opacity coefficient averaged over the rotation structure of the vibronic band of the given electron transfer of the molecule, i.e. it is supposed that for any frequency inside the band, the number of rotational lines is so large that characteristics of individual lines are not considered and the intensity distribution is thought to be continuous. Absorption in 27 bands of 11 molecules (CO, NO, SO, SiO, TiO, MgO, VO, BO, AlO, CN, MgH) is taken into account in the program (Pavlenko, Yakovina 1994). As far as allowance for convection is concerned, it was carried out according to the generally accepted mixing-length theory (Mihalas 1982; Kurucz 1970).

2.1. Program testing

For program approbation, model atmospheres of two stars were constructed: a class $A0$ star ($T_{eff} = 10000K$, $log\ g = 4.5$) and the Sun, for which the following parameters were adopted: $T_{eff} = 5780K$, $logg = 4.44$, $lg(Fe/H) = -4.49$.

Besides, the program was used for defining the parameters of the components of the binary system 41 Draconis (see p. 2.2). For A0 star a model atmosphere without molecular absorption and convection was calculated, for the Sun molecular bands and atmospheric convection were taken into account. The obtained temperature distribution was compared with Kurucz's models (1994), and for the Sun — with Fuhrmann's et al. (1997) models as well. The synthetic spectrum was also compared with spectra obtained using the models mentioned above.

The comparison of temperature distributions is given in Fig. 1. As is obvious, the $A0$ star according to our model in upper layers has a somewhat higher temperature than in Kurucz's model, which can be explained by the smaller number of lines taken into account, the absorption in which leads to both increase of the temperature of deep layers and cooling of external optically thin layers due to energy loss caused by radiation in lines.

However the difference in temperatures is small — it does not exceed 3% ($200K$) for $\tau_{ross} = 2 \cdot 10^{-5}$, it decreases to 0 when $\tau_{ross} = 0.05$ and remains at a level of 0.5% (50–70 K) and lower for $\tau_{ross} = 0.5 - 50$. By our model, in the deepest layers the temperature is lower than in Kurucz's model probably because of inadequate account of opacity. When $\tau_{ross} > 50$ the difference increases again to 200 K, but in relative units it makes at most 0.5%.

For the temperature distribution in the solar atmosphere, the situation is similar, with the exception that we see the dependence of temperature gradient on mixing length.

There is a small difference between our model and Fuhrmann's (1997) model for upper layers — the difference in temperatures reaches $5\%(180\,K)$ at $\tau_{ross} < 0.5$, decreasing to 30 K at $\tau_{ross} = 1$. However, the difference in temperature values of near-surface, and also of the deepest ($\tau_{ross} > 20$) layers exists for the published and widely used models as well. Thus, the temperature difference between Kurucz's and Fuhrmann's models reaches 200 K. This is connected with the difficulty of allowing for convection and molecular absorption, and besides — with essential dependence of temperature on adopted l/h ratio (the ratio of the homogeneous atmosphere height to the mixing length) especially in deep layers.

The parts of synthetic spectra calculated by the $SYNTH$ program (Kurucz 1994) using models being compared are displayed in Fig. 2. The fluxes differ from etalon ones for the A star by no more than 3%, the difference being on average 0.5%. For integral flux the difference is 0.08%. The spectra, calculated by models of Kurucz and ours for the Sun, differ in fluxes by at most 0.01, thus revealing complete coincidence.

Based on the models of the components of the binary system 41 Draconis (obtained by us and other authors), their synthetic spectra were constructed by the SYNTH program (Kurucz 1994), for comparison with observational data. Comparison of these spectra with the observed ones makes it possible to determine parameters of the real stars (p. 2.2).

As is seen from Fig. 1, 2, the synthetic spectra built on the basis of our model fit well with those based on the standard one, which proves correct functioning of the program.

2.2. Parameters of the components of the system 41 Draconis

The system 41 Draconis is a spectral and speckle-interferometric binary system with a period of 1247 days (Tokovinin 1995; Balega et al. 1997; Tokovinin et al. 2003).

Physical parameters of the system's components were analysed from echelle spectra obtained (April 2001) with the BTA NES spectrograph (Panchuk et al. 2002) and processed by D. Kudryavtsev. We used 37 unblended lines of different heavy elements. The difference of radial velocities made it possible to conduct measurements for each component of the system separately (see Appendix). Since the resulting spectrum is the sum of spectra of the components, the directly measured equivalent widths of lines do not

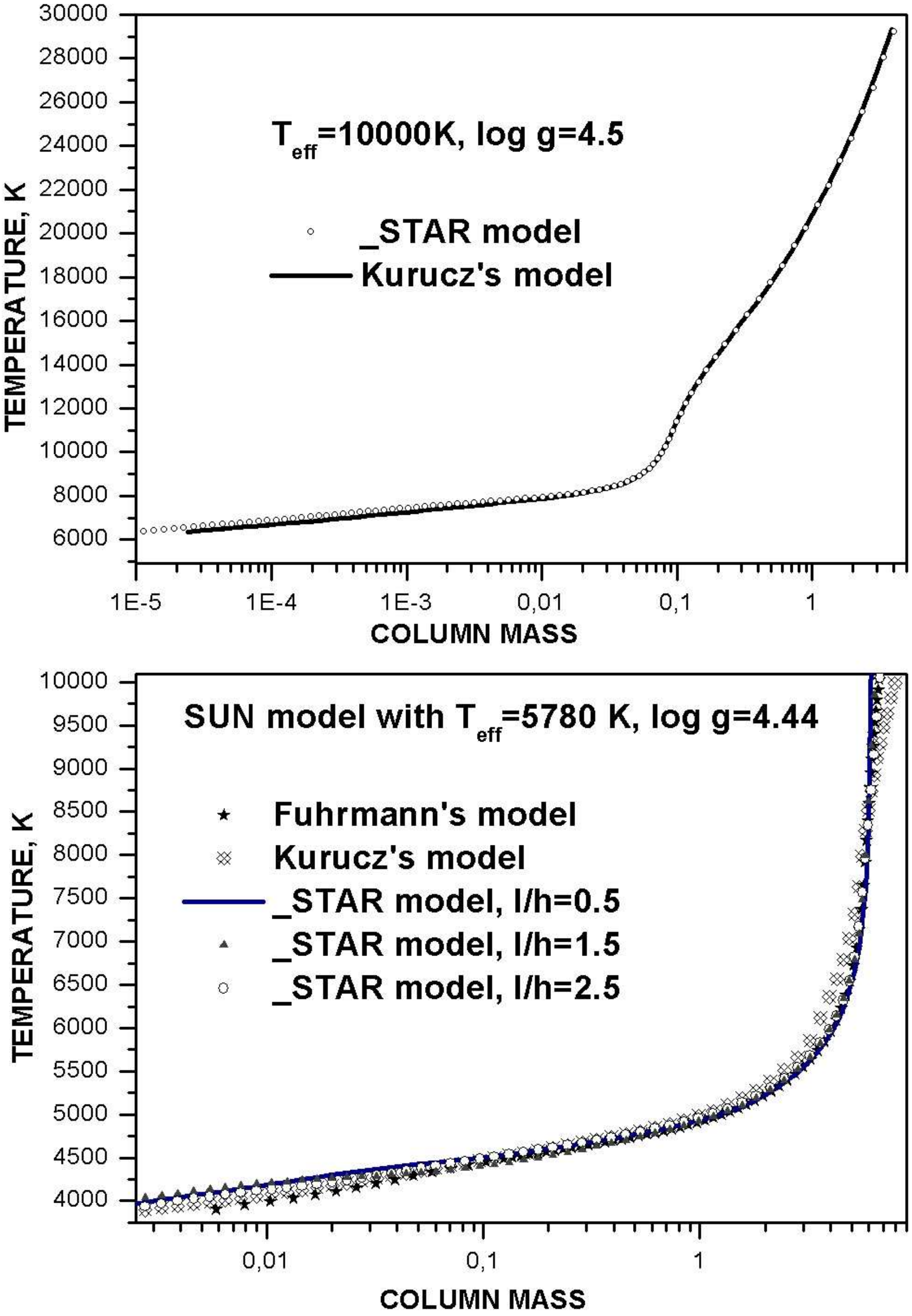

Figure 1: *Comparison of temperature distributions in star atmosphere with* $T_{eff} = 10000, log\ g = 4.50$ *in Kurucz's (1994) model and in our model (at the top). The comparison of temperature distributions for the Sun atmosphere (at the bottom). Kurucz's (1994) model with* $l/h = 2$*, Fuhrmann's (1997) model, calculated for the* $l/h = 0.5$*, and our models calculated for different* l/h *values are given.*

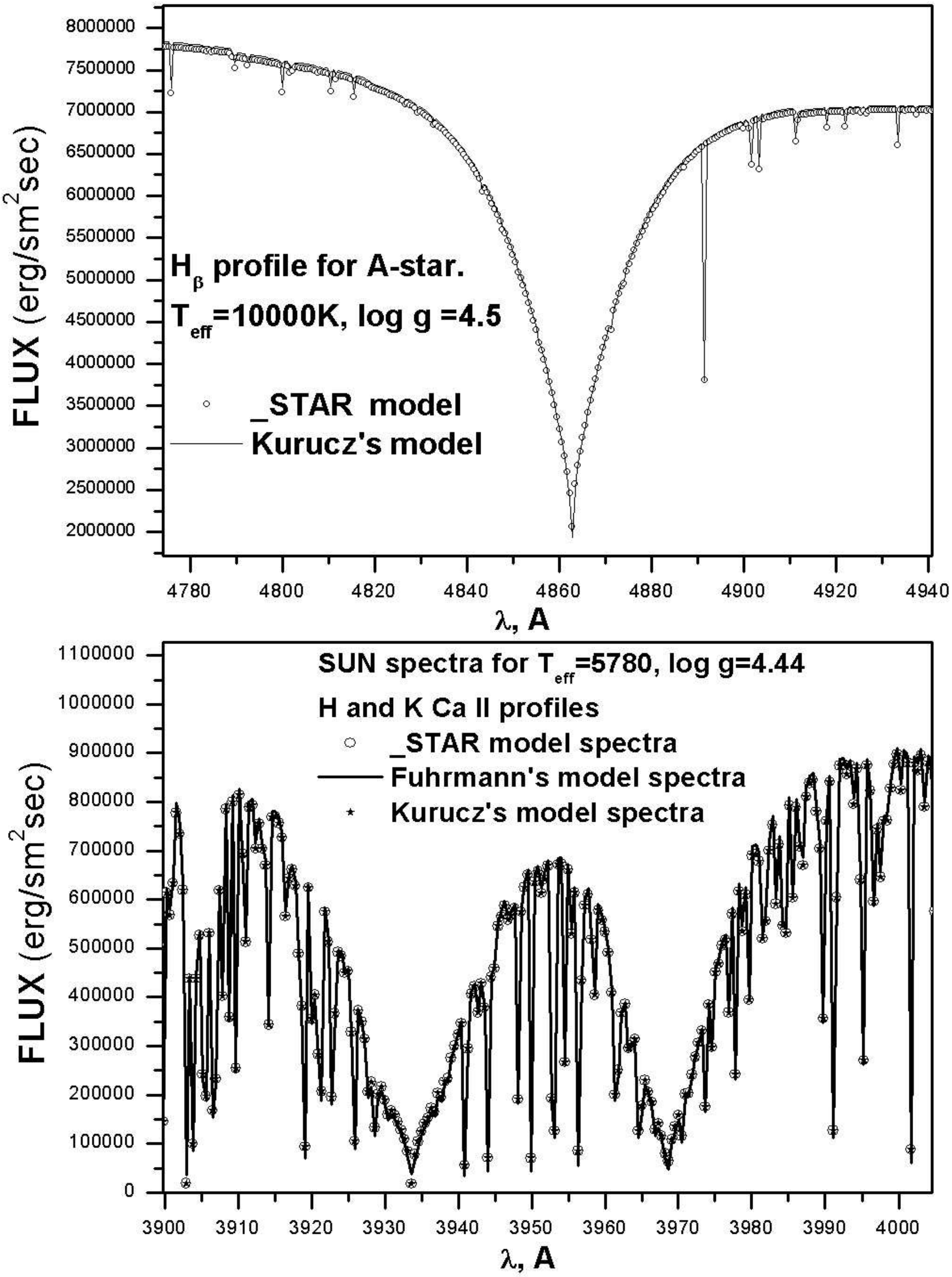

Figure 2: *Comparison of synthetic spectra in* H_β *line region for the star with* $T_{eff} = 10000, log\ g = 4.50$ *in Kurucz's (1994) model and in our model (at the top). Comparison of the Sun synthetic spectra in H and K CaII lines region in Kurucz's (1994), Fuhrmann's (1997) models for* $l/h = 0.5$ *and in our model — for* $l/h = 0.5$ *(at the bottom).*

Table 1: *Parameters of the components of the system 41 Draconis. [1] — Balega et al. (2001), [2] — Al-Wardat et al. (2002)*

Parameter	This work	[1]	[2]
$T_{eff}(a),\ K$	6540 ± 100	6500	6100
$T_{eff}(b),\ K$	6570 ± 100	6500	6100
$log\ g(a),\ dex$	4.12 ± 0.08	3.99	3.86
$log\ g(b),\ dex$	4.15 ± 0.08	4.11	4.01
$Z(a),\ dex$	0.031 ± 0.002		
$Z(b),\ dex$	0.030 ± 0.002		
$VsinI(a),\ km/sec$	8.05 ± 0.5		
$VsinI(b),\ km/sec$	8.07 ± 0.5		

correspond to the values obtained from the model spectra of a single star. Relation between the real equivalent widths and the widths observed can be defined as:

$$EW_a = EW_a^{obs}(1+k),$$
$$EW_b = EW_b^{obs}(1+k)/k,$$

where $k = E_{\lambda,b}/E_{\lambda,a}$ is the relation of the fluxes of the components at a given wavelength. Of course, such an approach is possible with a sufficient difference between radial velocities, only if lines of the components are reliably resolved.

For the system 41 *Dra* $k = 0.65$ for $\lambda = 5000$ Å and is practically independent of the wavelength.

Model spectra were derived by the program *SYHTH* on the basis of the grid of models calculated by the complex _STAR. The set of parameters is defined by comparing observed equivalent widths with the model ones using the least-squares method, which results in their best fit. Such a method excludes effect of uncertainty in axial rotation velocity, which changes the line profile, but not its equivalent width. Thus T_{eff}, *log g* and metallicity Z were defined. The projection of the axial rotation velocity on the line of sight $V \sin i$ was defined after the determination of model parameters by comparing line FWHM calculated for different rotation velocities with FWHM observed. The obtained parameters were compared with the results of investigation of this system by other authors (Table 1).

As we can see, within the measurement errors, the parameters that we defined coincide with the results of other authors obtained earlier (and also having errors), and this gives promise that it is possible to use our program to define parameters of both single stars and components of multiple systems.

3. Conclusion

In this paper we present a model atmosphere program *_STAR*, which is a development of the complex *ATLAS* 5 (Kurucz 1970). It allows making calculation of LTE model atmospheres, taking into consideration 500000 absorption lines for any chemical composition, which is an important condition for modeling of peculiar star atmospheres.

The program passed testing and showed good correspondence between results obtained with its help and widely used models.

The determination of the model parameters of the system 41 Draconis also demonstrated good agreement with data of other authors. Those who wish to obtain primary files can contact the authors at the following addresses: gilgalen@yandex.ru (R.Ya.Zhuchkov), vals@ksu.ru (V.F.Suleymanov, V.V.Shimanski).

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References

Al-Wardat M., 2002, Bull. Spec. Astrophys. Obs., **53**, 51

Balega I.I., Balega Yu.Yu., Falcke H., Osterbart R., Reinheimer T., Schöller M., Weigelt G., 1997, Pis'ma Astron. Zh., **23**, 199

Balega Yu.Yu., Leushin V.V., Pluzhnik E.A., 2001, Bull. Spec. Astrophys. Obs., **51**, 61

Fuhrmann K., Pfeiffer M., Frank C., Reetz J., Gehren T., 1997, A&A, **323**, 909

Kurucz R.L., 1970, SAO Special Report, **309**

Kurucz R.L., 1994, CD-Roms's

Mihalas D., 1982, Star atmospheres, **1, 2**, Moscow: Mir

Panchuk V.E., Piskunov N.E., Klochkova V.G., Yushkin M.V., Ermakov S.V., 2002, Preprint SAO, No.169

Pavlenko Ya.V., Yakovina A.A., 1994, Astron. Zh., **76**, 863

Tokovinin A.A., 1995, Pis'ma Astron. Zh., **21**, 286

Tokovinin A.A., Balega Yu.Yu., Pluzhnik E.A., Shatsky N.I., Gorynya N.A., Weigelt G., 2003, A&A, **409**, 245

Shimanskaya N.N., 2001, PhD Thesis, Kazan

4. Appendix

Table 2: *List of lines for which the measurements were taken, values of their equivalent widths and half-widths for a and b components, respectively*

Element	λ(Å)	EW_a(Å)	$FWHM_a$(Å)	EW_b(Å)	$FWHM_b$(Å)
Y II	4883.68	0.067	0.097	0.234	0.215
FE I	4903.30	0.122	0.118	0.290	0.280
Ni I	4904.41	0.078	0.078	0.260	0.275
Fe I	4988.96	0.074	0.082	0.235	0.236
Fe I	5044.21	0.085	0.067	0.280	0.252
Fe I	5049.82	0.116	0.117	0.255	0.274
Cu I	5105.53	0.036	0.043	0.180	0.228
Ni I	5155.76	0.050	0.070	0.170	0.238
Fe I	5159.05	0.066	0.061	0.247	0.237
Fe I	5162.30	0.117	0.118	0.288	0.271
Ti II	5211.54	0.056	0.055	0.252	0.250
Fe I	5228.40	0.083	0.053	0.356	0.259
Fe II	5234.63	0.098	0.097	0.248	0.268
Fe I	5281.77	0.127	0.128	0.265	0.315
Fe I	5288.52	0.046	0.049	0.247	0.240
Fe I	5322.04	0.052	0.049	0.270	0.245
Fe I	5324.18	0.183	0.155	0.312	0.295
Ti II	5336.77	0.063	0.070	0.215	0.211
Cr I	5348.31	0.067	0.069	0.220	0.241
Ti II	5381.01	0.079	0.068	0.295	0.249
Fe I	5383.37	0.125	0.132	0.265	0.273
Fe I	5391.45	0.076	0.090	0.277	0.316
Fe I	5393.17	0.111	0.114	0.289	0.288
Fe I	5398.27	0.063	0.057	0.280	0.248
Mn I	5399.50	0.024	0.023	0.239	0.236
Fe I	5410.91	0.112	0.125	0.290	0.313
Fe I	5445.04	0.095	0.090	0.254	0.248
Fe I	5464.27	0.046	0.038	0.233	0.263
Fe I	5506.78	0.104	0.095	0.252	0.214
Y II	5509.93	0.079	0.070	0.380	0.348
Fe I	5522.45	0.029	0.029	0.204	0.220
Sc II	5526.79	0.087	0.095	0.250	0.281
Fe I	5569.62	0.111	0.109	0.257	0.247
Fe I	5576.09	0.090	0.092	0.252	0.249
Ni I	5578.71	0.050	0.044	0.301	0.264
Ca I	5581.95	0.072	0.082	0.218	0.245
Ca I	5590.12	0.071	0.073	0.237	0.262