Spectrum synthesis for magnetic, chemically stratified stellar atmospheres

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Abstract. Modern investigations of magnetic chemically peculiar stars reveal a variety of complex processes in their atmospheres. Realistic spectrum synthesis modelling of these objects has to take into account anomalous chemical composition, strong magnetic field and chemical stratification. These effects complicate calculation of theoretical spectra, especially when one has to deal with a large number of lines and wide spectral regions. To overcome the formidable problem of comparing model and observed spectra for magnetic chemically peculiar stars, a new suite of spectrum synthesis programs was developed. Here we describe in detail the synthesis codes, SYNTH3 and SYNTHMAG and present examples of their application to various aspects of the peculiar-star surface phenomena. The new codes proved to be reliable tools for the line identification, magnetic field determination, chemical abundance and stratification analysis.

Key words: line: profiles – polarization – radiative transfer – stars: chemically peculiar – stars: magnetic fields – stars: atmospheres

1 Introduction

Recent major improvements in the quality of spectroscopic observations stimulated a surge of interest in detailed model atmosphere and chemical abundance studies of magnetic stars. Modern spectrographs, such as UVES at the ESO 8-m VLT at Paranal, HARPS at the ESO 3.6-m telescope at La Silla, or the NES instrument at the SAO 6-m telescope, can now provide $S/N > 300$, wide spectral coverage echelle spectra of moderately faint stars at the resolving power of $\lambda/\Delta\lambda = 4\times10^4$–$10^5$. Publicly accessible data archives assist in distributing these spectra to an astronomical community far wider than the co-investigators on the original observing proposals or scientists from the countries that own the telescopes and instruments.

Availability of the new observational material has to be matched by the corresponding development of the new analysis techniques, capable of handling large spectral regions and large number of lines without compromising accuracy. The complex chemistry of chemically peculiar (CP) stars, coupled with the prominence of the magnetic field and chemical stratification effects, implies that any realistic analysis of the atmospheres of these stars must be partly or entirely based on the method of spectrum synthesis. Moreover, to deduce accurate chemical abundances, theoretical computations must properly account for the transfer of polarized radiation through the chemically inhomogeneous stellar atmosphere. Numerical schemes implemented in the codes have to be stable against rapid variation of the equilibrium model structure and opacity, associated with the chemical clouds, located at different atmospheric heights.

Several computer codes for modelling the time series of Stokes parameter spectra were developed in the past (Wade et al. 2001), but they are typically constrained to the analysis of short wavelength regions and are not thoroughly tested with the chemically stratified atmospheres. The lack of general-purpose spectrum synthesis codes, suitable for modelling magnetic, chemically stratified stellar atmospheres, stimulated development of new tools and major improvement of the existing, widely used software. In this paper we describe the current status and recent updates of our two spectrum synthesis codes: SYNTHMAG (magnetic spectrum synthesis) and SYNTH3 (computation of non-magnetic stellar spectra). The former code represents a major revision and improvement of the early magnetic spectrum synthesis code by Piskunov (1999), whereas the latter supersedes the well-known SYNTH code (Piskunov 1992).

2   Physical foundations

SYNTHMAG and SYNTH3 are designed to calculate spectra emerging from the static, plane-parallel, one-dimensional model atmosphere. The Local Thermodynamical Equilibrium assumption is used throughout. These approximations are adequate for a wide range of stars in the Main Sequence band. In practice, the codes were successfully used to model stars in the range of spectral classes from early-B to late-M.

2.1   Opacities

The polarized radiation is fully characterized by the Stokes vector $\boldsymbol{I} = \{I, Q, U, V\}^{\dagger}$, where the Stokes parameters are defined according to Shurcliff (1962). The SYNTHMAG code solves the polarized radiative transfer equation in the form

$$\mu \frac{d\boldsymbol{I}}{dm} = -\mathcal{K}\boldsymbol{I} + \boldsymbol{J}, \tag{1}$$

where m denotes the column mass scale, which is used for tabulation of model atmospheres, and $\mu \equiv \cos\theta$ is the cosine of the angle between line of sight and the local surface normal. For the sake of brevity, here we omit complete expressions of the elements of the absorption matrix $\mathcal{K}$ and of the emission vector $\boldsymbol{J}$, since this was discussed in detail by Piskunov & Kochukhov (2002).

In calculating the metal line opacities, SYNTHMAG takes into account Zeeman or Paschen-Back splitting patterns specified in the input line list. The absorption and anomalous dispersion profiles for each Zeeman component are described by the Voigt and Faraday-Voigt function, respectively. Radiative, van der Waals and Stark broadening is calculated according to the damping parameters provided in the line list or using classical expressions (Gray 1992). The chemical and ionization equilibrium is calculated for a prescribed vertical distribution of abundances. Absorption profiles of all lines contributing to a given wavelength are summed and multiplied by the trigonometric functions of the angles γ and χ, which define orientation of the local field vector with respect to the line of sight. The resultant coefficients enter the absorption matrix $\mathcal{K}$.

The hydrogen line opacity is determined with the routines developed by Barklem et al. (2000). The Stark broadening tables of Stéhle (1994) are used to account for the linear Stark effect. Self-broadening of hydrogen lines (Barklem et al. 2000) is also included. An optional module permits improved calculations of the overlapping lines of the higher hydrogen series members with the occupation probability formalism of Daeppen et al. (1987) and Hubeny et al. (1994).

The Stark broadening parameters of the neutral He lines are computed following Dimitrijevic & Sahal-Brechot (1984) and Freudenstein & Cooper (1978).

The continuous opacity calculation in our spectrum synthesis codes is based upon the routines adapted from the ATLAS9 code (Kurucz 1993). We include absorption due to the bound-free and free-

free transitions of H I, H_2^+, H^-, He I, He II, different metal ions, He^- free-free, Rayleigh scattering for H I and He I, and electron scattering.

Opacity calculations in SYNTH3 are similar to those of SYNTHMAG, except that a non-magnetic version of Eq. (1) is used and unpolarized radiation is computed using the usual scalar opacity coefficients. It was verified that the line profiles of SYNTH3 are identical to calculations with SYNTHMAG if magnetic field strength is set to zero.

2.2   Ionization and molecular equilibrium

Ionization and molecular equilibrium in SYNTH3 and SYNTHMAG is obtained with the advanced equation of state solver written by N. Piskunov. This code represents a modified and expanded version of the routine described in Valenti et al. (1998). The solver includes the treatment of ≈ 200 diatomic and polyatomic molecules and has been thoroughly tested against similar routines of the MARCS and PHOENIX model atmosphere codes for temperatures from $\sim 10^5$ K down to a few hundred K.

Atomic partition functions are calculated using the tables given in the PFSAHA subroutine of the ATLAS9 code (Kurucz 1993). For a number of heavy elements, especially rare-earths, updated partition functions of Cowley & Barisciano (1994) and Sneden (2002) are incorporated. For calculations of the ionic populations we typically take into account 6 ionization stages for light elements, 4 stages for the iron-peak group and 3 stages for heavy elements.

For diatomic molecules the partition function information is taken from Sauval & Tatum (1984) and Irwin (1987). For polyatomic molecules, the data from Irwin (1988) are used.

2.3   Magnetic field

Detailed structure of the stellar magnetic field geometry is best studied with the time-resolved spectropolarimetric observations using Doppler imaging (Piskunov & Kochukhov 2002) or fitting parameters of the multipolar field models (Khalack & Wade 2006). On the other hand, the main purpose of SYNTHMAG is to properly account for the Zeeman broadening and splitting in a wide wavelength region analysis of the unpolarized spectra of magnetic stars. Information content of a few unpolarized stellar observations, available for the majority of CP stars, is usually insufficient to constrain even the most simple model of the field geometry, especially when no rotational modulation can be detected. This is why the common approach of expanding the field structure in spherical harmonics is poorly constrained and one has to resort to a simplified field model, characterized by a small number of free parameters. Following this ideology, the SYNTHMAG code calculates the local Stokes $IQUV$ spectra for a set of angles between the line of sight and local surface normal assuming that i) the field is axisymmetric with respect to the line of sight and ii) the field structure is homogeneous and is defined by the three vector components: radial, meridional and azimuthal field (see Fig. 1). This is essentially equivalent to approximating the field strength distribution with a single value — an approach which works surprisingly well for many slowly rotating CP stars.

3   Numerical details

Both the SYNTHMAG and SYNTH3 programs are written in Fortran 77, which ensures portability to all major computer platforms and straightforward interfacing with alternative software modules. The codes use standard BLAS and LAPACK routines, but do not depend on commercial or proprietary software libraries. Up to now, the codes were compiled and successfully used on the SunOS and HP-UX versions of the Unix operating system, on Mac OSX and Linux.

In the standard mode, SYNTH3 computes intensity by solving numerically the scalar radiative transfer equation for a set of (typically) seven μ angles. SYNTHMAG proceeds similarly, but solves the vector polarized RT equation and derives Stokes $IQUV$ profiles for a given local magnetic field.
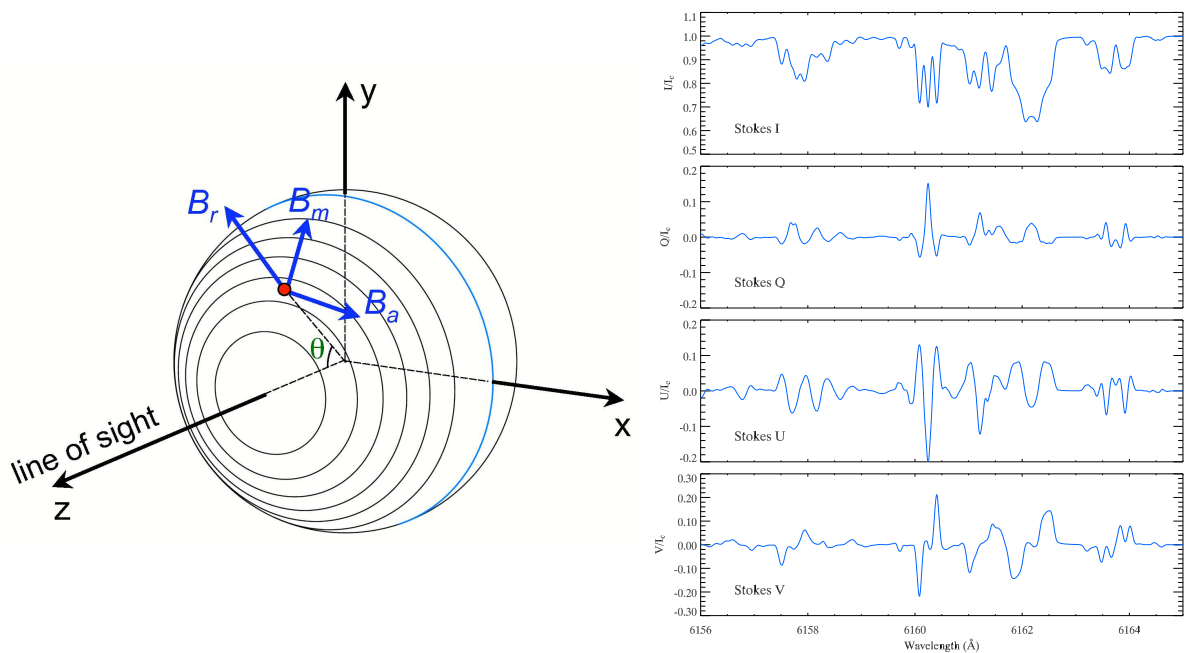
Figure 1: *Left panel*: magnetic field geometry adopted in SYNTHMAG. The field structure is symmetric with respect to the line of sight (*z*-axis). The three magnetic vector components, B_r, B_a, B_m, describe the radial, meridional and azimuthal field in the stellar reference frame. Transformation of the local field vector to the observer's coordinate system xyz depends on the angle θ of each of the seven annular zones employed for calculation of the disk-integrated profiles. *Right panel*: typical four Stokes parameter disk-center SYNTHMAG calculations for $B = 10$ kG and $T_{\mathrm{eff}} = 7700$ K.

Each code does the following set of operations:

- Reading the input model atmosphere (krz format) and atomic/molecular line list in the VALD format (Kupka et al. 1999). For SYNTHMAG the input line list also contains information on the strength and splitting of the Zeeman components for each line. Depth dependence of chemical abundance, magnetic field strength or microturbulent velocity can be specified in the input model atmosphere file.

- Concentrations of ions and molecules are computed with the equation of state module described above. For each layer in the model atmosphere we calculate continuous and line center opacities and the Voigt function parameters. The depth grid is refined if necessary.

- Intensity at several limb angles is computed with the help of formal polarized (or scalar for SYNTH3) radiative transfer algorithm, using precomputed line-center opacities. The wavelength grid is refined to obtain an accurate description of the line profile shapes.

- Intensity profiles are broadened for a given projected rotational velocity and macroturbulence. The resultant profiles are combined to form the disk-integrated spectra.

3.1   Integration of the radiative transfer equation

The polarized radiative transfer equation (1) is solved on discrete vertical grid using the Diagonal Element Lambda Operator (DELO) formal solver, introduced by Rees et al. (1989). In our spectrum synthesis codes we employ a modified DELO algorithm, which utilizes a parabolic approximation of the source function (Socas-Navarro et al. 2000). Piskunov & Kochukhov (2002) have compared
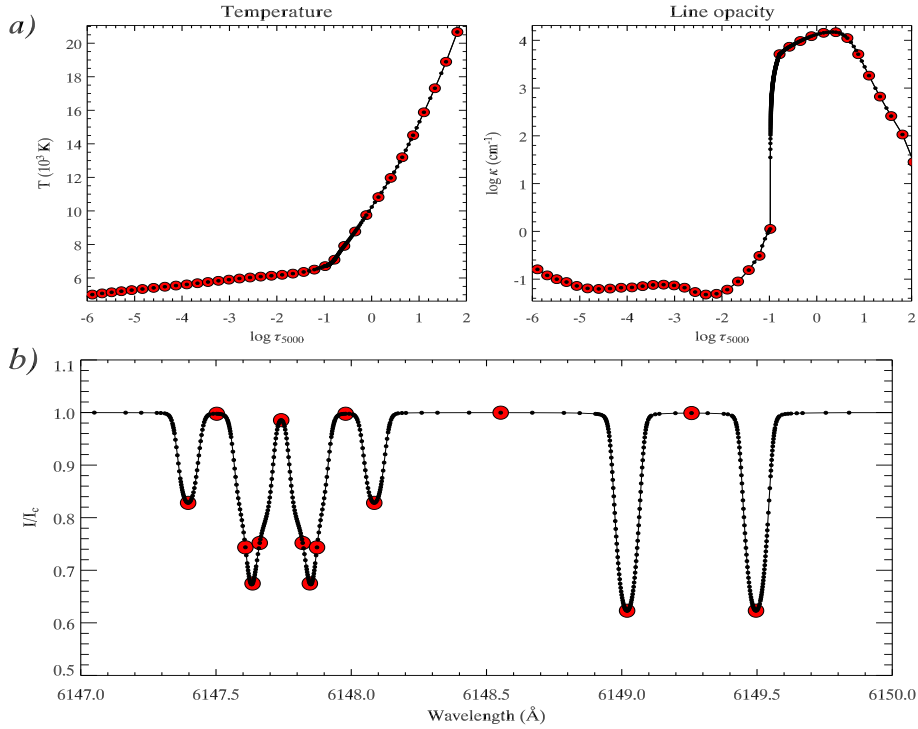
Figure 2: Illustration of the adaptive grid refinement in `SYNTHMAG`. **a)** Extra layers are added in the model atmosphere if vertical variation of the total opacity is too fast. Large symbols show the original discretization of the model; small symbols illustrate the final depth grid. **b)** Refinement of the frequency grid. Initially spectra are calculated for the centers of Zeeman components and for the wavelengths in between (large symbols). More points (small symbols) are added until the line profile shapes are described with sufficient accuracy.

several widely used polarized radiative transfer algorithms and found that the quadratic DELO method is superior in terms of speed and accuracy to the original DELO solver and to all other polarized radiative transfer schemes. For typical `ATLAS9` model atmospheres of the Main Sequence B-F stars the accuracy of Stokes parameter calculation with the DELO algorithm is $\sim 10^{-4}$.

Rapid variation of abundances with height in the atmospheres of chemically peculiar stars poses further challenges to a radiative transfer solver. The latter has to provide accurate spectra for minimum number of layers in the model atmospheres and, at the same time, be robust against steep variation of the line opacity resulting from chemical stratification. In the recent paper Kochukhov et al. (2006) investigated performance of different scalar radiative transfer algorithms for chemically stratified stellar atmospheres. These numerical experiments showed that direct intensity integration implemented in Kurucz (1993) codes is remarkably stable and performs well for atmospheres with chemical stratification. However, this algorithm cannot be extended to polarized radiation and for this reason it is not used in our codes. The quadratic DELO scheme achieves acceptable accuracy of $\sim 10^{-3}$ for the atmospheres with large abundance gradients if extra vertical grid points are added between the layers where opacity changes rapidly.

3.2 Spectrum synthesis with adaptive grids

To achieve required precision with the least amount of computations, adaptive grids are extensively used in `SYNTHMAG` and `SYNTH3`. At the stage of precalculation of the line-center opacities, both codes consider the vertical gradient of the monochromatic optical depth. If variation of the optical

depth exceeds a given threshold, an extra layer is added in the model structure. Tabulated model atmosphere quantities are obtained for additional layers with the help of spline interpolation. The procedure of the depth grid refinement is essential to obtain accurate spectra for the chemically stratified atmospheres. An example of the depth grid refinement for cool Ap-star atmosphere with a strong vertical gradient of the iron abundance is presented in Fig. 2a.

Most spectrum synthesis codes calculate line profiles on a wavelength grid defined by a fixed wavelength step. This leads to computation of excessive number of continuum points with no useful information. On the other hand, a coarse equidistant grid may not allow one to resolve details of the line profile shapes. SYNTHMAG and SYNTH3 avoid this difficult compromise between the line profile accuracy and amount of computations by using adaptive wavelength grid. At the first step, intensity is calculated at the centers of spectral lines or Zeeman components, if the magnetic field is present. Then spectral points between each pair of the original wavelengths are synthesized. Computed intensity is compared with the results of linear interpolation and further frequency points are added if the discrepancy between interpolated and computed spectra exceeds a given threshold. In this way, more points are calculated for the regions with rapid variation of opacity, whereas the wavelength step remains relatively large for continuum regions (see Fig 2b). Using this procedure, we obtain theoretical spectra at infinite resolution, performing a factor of 10 to 50 less computations to achieve the same accuracy as in the synthesis with a sufficiently fine equidistant wavelength grid.

3.3   Disk integration

The final step of the spectrum synthesis calculation with SYNTHMAG and SYNTH3 is integration of the local Stokes parameter/intensity spectra to obtain stellar flux profiles. We use an external procedure, compatible with both the SYNTHMAG and SYNTH3 output files, to perform the disk integration.

In the default mode, the local intensity and Stokes parameter spectra are calculated for seven annular surface zones, chosen in such a way that their projected surface areas are equal (see left panel in Fig. 1). Numerical experiments have demonstrated that this discretization of the stellar surface is sufficient for computation of high-precision unpolarized spectra. On the other hand, due to substantial variation of the shape and intensity of the Stokes QUV local profiles over the stellar surface in any realistic magnetic field configuration, co-addition of seven linear and circular polarization local spectra provides only a rough estimate of the signal expected in the QUV disk-integrated spectra.

Intensity spectra are convolved with the appropriate rotational and radial-tangential macroturbulence broadening profiles (Gray 1992) and then added with equal weights. This assumes spherically symmetric star, covered by a homogeneous magnetic field. We note, however, that SYNTHMAG and SYNTH3 are, in fact, independent of the latter assumptions of the disk integration and can be used to supply intensity spectra for a more sophisticated disk integration procedure. For instance, different sets of intensity spectra can be combined to simulate observations of rotationally distorted stars, stars covered with chemical, temperature or magnetic spots, etc. Below we give an example of such an advanced usage of SYNTHMAG for calculation of the Zeeman resolved spectral lines corresponding to dipolar field geometry.

3.4   Reconstruction of chemical stratification

Early attempts to deduce vertical chemical stratification in the atmospheres of Ap stars were based on the trial-and-error method (Ryabchikova et al. 2002). Abundances in the upper and lower parts of the stellar atmosphere were manually adjusted to fit the line profile shapes and to remove a discrepancy between the strength of lines of different excitation potential, equivalent width and ionization stages. We have recently developed an automatic procedure, DDAFit, to find chemical abundance gradients from observed stellar spectra (Ryabchikova et al. 2005). The DDAFit script is
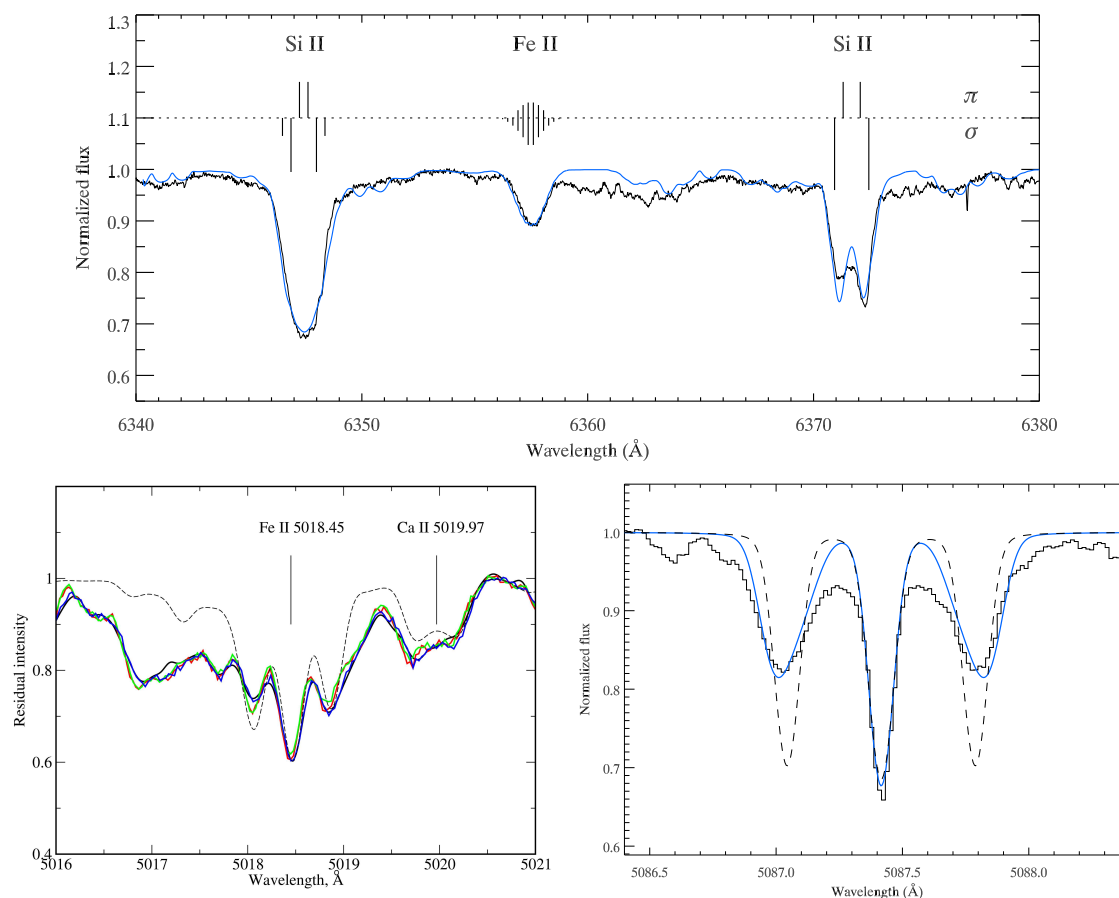
Figure 3: Examples of the `SYNTHMAG` modelling of the spectra of magnetic CP stars. *Top panel*: comparison between observations of the red Si II doublet at λ 6347 and 6371 Å and spectrum synthesis for HD 137509 – the star with second-largest field known ($\langle B \rangle$ = 29 kG, Kochukhov 2006). *Bottom left panel*: detection of the Zeeman resolved components in the Fe II 5018 Å line in the spectrum of cool Ap star HD 178892 (Ryabchikova et al. 2006a). In this plot solid lines show observations obtained with the NES instrument at the SAO 6-m telescope, whereas dashed line shows `SYNTHMAG` calculation for $\langle B \rangle$ = 17.5 kG. *Bottom right panel*: observations (histogram) of the Y II 5087 Å line in the strongly magnetic cool Ap star HD 154708. Usual `SYNTHMAG` calculation for $\langle B \rangle$ = 24 kG (dashed line) is compared with the result of combining spectra for a dipolar-like distribution of the field strength in the range from 29 to 16.5 kG (solid line).

written in IDL and provides an optimization and visualization interface to the spectrum synthesis calculations with `SYNTHMAG` and `SYNTH3`. Vertical abundance distributions are described with the four parameters: chemical abundance in the upper atmosphere, abundance in deep layers, the vertical position of abundance step and the width of the transition region where chemical abundance changes between the two values. All four parameters can be optimized simultaneously with the Levenberg-Marquardt least-squares fitting routine (Bevington & Robinson 1992) and based on observations of unlimited number of spectral regions, possibly using different weights in accordance to the quality or relative importance of the observations of particular spectral features. The program derives one chemical stratification profile at a time, but is able to account for any number of fixed stratified abundances.

4   Applications

4.1   Magnetic stars

SYNTHMAG was used in a number of recent studies of magnetic Ap stars. In such analyses polarized radiative transfer calculations are essential to derive accurate abundances, resolve contributors to complex blends and to measure magnetic field strength.

Fig. 3 illustrates application of SYNTHMAG to three different chemically peculiar stars with strong magnetic field. For the Si-peculiar Bp star HD 137509 (Kochukhov 2006) we show comparison of observations and theoretical spectra in the region of the Si II doublet at λ 6347 and 6371 Å. Strikingly different profile shapes of the two, otherwise similar, lines can be traced to the different Zeeman splitting structure. Resolved Zeeman components in the Si II 6371 Å line indicate $\langle B \rangle = 29$ kG, which is a second-largest field ever observed in a non-degenerate star. This very large field strength is confirmed by the spectrum synthesis of other metal lines.

We also show application of SYNTHMAG to the analysis of HD 178892 – a star discovered by the magnetic surveys at the SAO 6-m telescope (Elkin et al. 2002). The follow up high-resolution spectroscopy with NES (Ryabchikova et al. 2006a) reveal resolved Zeeman components in many lines, for example Fe II 5018 Å shown in Fig. 3. Low $T_{\rm eff}$, strong magnetic field ($\langle B \rangle = 17.5$ kG) and relatively short rotation period make HD 178892 an excellent candidate for a detailed analysis of the horizontal structure of magnetic field and chemical abundance spots.

HD 154708 is another unique cool Ap star, showing very strong magnetic field ($\langle B \rangle = 24.5$ kG, Hubrig et al. 2005). Recent time-series observations at ESO suggest the presence of low-amplitude p-mode pulsations in this star (Kurtz et al. 2006). Due to an extremely slow rotation, Zeeman components are fully resolved for many spectral lines in HD 154708. The field is so strong however, that the standard SYNTHMAG approximation of the surface field strength distribution with a single value of the field modulus fails (see Fig. 3). This is evident from the comparison of spectrum synthesis and observed profiles of the σ components in the Zeeman split triplet lines: σ components are broader and shallower in observations, indicating a non-negligible surface scatter of the field strength. This situation can be addressed with a straightforward extension of the spectrum synthesis with SYNTHMAG. Fig. 3 shows that a much better agreement with observations can be achieved if the stellar flux profiles are produced from a set of SYNTHMAG computations for different field strengths, corresponding to the $B_{\rm p} = 30$ kG dipolar field topology.

4.2   Chemically stratified atmospheres

Both SYNTHMAG and SYNTH3 can calculate spectra for the prescribed inhomogeneous vertical distribution of chemical elements. Parameters of the simple step-function distribution of abundances with depth can be adjusted with the help of the DDAFit script described above.

A number of recent chemical abundance analyses of Ap stars accounted for chemical stratification in the spectrum synthesis with SYNTHMAG and SYNTH3 and obtained vertical distributions of selected elements using the DDAFit procedure. Fig. 4 illustrates application of SYNTHMAG to the problem of deriving Fe stratification in the strongly magnetic Ap star HD 144897 (Ryabchikova et al. 2006b). Another example of employing SYNTH3 and DDAFit to the chemical stratification modelling can be found in Ryabchikova et al. (2005).

5   Conclusions

We have developed a new family of spectrum synthesis codes for modelling the spectra of stars with various atmospheric parameters and chemistry. The codes SYNTHMAG and SYNTH3 can be used to calculate line profiles of normal stars with different $T_{\rm eff}$, as well as peculiar stellar objects with
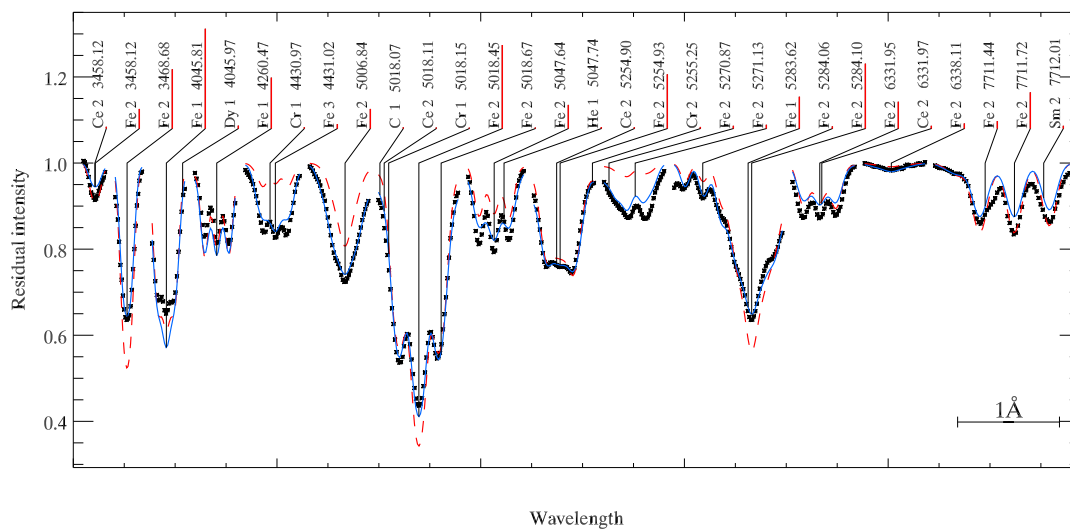
Figure 4: Spectrum synthesis calculation for chemically stratified atmosphere of the Ap star HD 144897 (Ryabchikova et al. 2006b). Symbols show observed line profiles. Dashed curve illustrates theoretical spectrum for constant Fe abundance. A better fit to observations (solid line) could be achieved by taking into account vertical stratification of Fe.

strong magnetic fields, non-solar chemical composition and vertical chemical abundance gradients. Inclusion of the molecular opacities and employment of the general equation of state solver permits application of our codes to a wide variety of stars across the H-R diagram.

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