# Non-LTE Line Formation for Iron-Group Elements in A Supergiants

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**Abstract.** Model atoms for Fe II and Ti II are introduced and first results are presented. Whereas the non-LTE effects are small for Fe II, preliminary results for Ti II suggest a potential for non-LTE effects. Our line-formation techniques can now take the effects of mass loss into account. The strongest lines of Fe II are obviously wind affected and can be reproduced by our calculations.

## 1. Introduction

New telescopes with excellent detectors provide spectra of hitherto unknown quality. They have made the step to galaxies at distances greater than those of the Magellanic Clouds a reality. In these galaxies A supergiants, with their high intrinsic visual brightness, are prime targets for spectroscopy, and therefore the quantitative analysis of A supergiants has become an active field of research. Kim Venn, together with members of the Munich group, has been able to provide excellent metal abundances for several galaxies, allowing metallicity gradients and chemical evolution to be studied (see Venn et al. 1998 and references therein). Also, such work is needed to calibrate the wind-momentum–luminosity relation (WLR), which can be used as a distance indicator (Puls et al. 1996).

One aim of the work presented in this paper is to be able to perform similar analyses for galaxies at even greater distances. Spectra for such objects will not be obtainable at the same same S/N ratio and/or dispersion as used in the work carried out so far. Therefore, one of our goals is to provide reliable methods and models to perform quantitative spectroscopy on A supergiants at distances where the current methods will fail. Noisier spectra, at lower resolutions, will require the strongest lines of any species to be considered rather than the weakest as is currently the case. Thus, we will have to be able to describe adequately non-LTE effects, and also the effects of mass loss on the metal lines under consideration. For the most extended objects even the effects of spherical extension may come into play.

Most of the strongest lines will be on the damping part of the curve of growth and therefore will not show the same strong dependence on abundance as the weaker lines, while at the same time they are strongly affected by microturbulence and a velocity field. Non-LTE effects will have to be considered as well, especially since the brightest targets will be the most extended, and therefore lowest-density, objects.

The ultimate aim is to provide a list of strategic lines which will provide abundances and microturbulent velocities at the best obtainable accuracy. Before such work can be tackled, the effects of all the processes mentioned above will have to be disentangled. Thus, we will first concentrate on the beautiful high-resolution, high-S/N spectra currently available for 'nearby' objects, in order to fine-tune the diagnostics required for the next step.

This paper presents some of the first results of the project outlined above. In the next section the model atoms for Fe II and Ti II are described and the methods used in the line-formation calculations are discussed. Some first results follow, and a summary and outlook conclude the presentation.

## 2. Models and Methods

### 2.1. The Model Atoms

So far, model atoms for Fe II and Ti II have been completed. They include all observed levels as given by Sugar & Corliss (1985). Figure 1 shows the Grotrian diagram containing all transitions which are included in the calculation of the populations of Ti II, which is the smaller of the two ions described here. Note that the individual levels are packed into LS-coupling terms for this step.

Whenever possible, the most accurate atomic data available have been used. For Fe II we have:

- $f$ values from Nahar & Pradhan (1995) and Kurucz (1988);
- photoionization data from Nahar (personal communication; note that the full resonance structure is accounted for);
- collisional bound-bound cross-sections from Zhang & Pradhan(1995)

and for Ti II:

- $f$ values from Kurucz (1988);
- photoionization cross-sections from a calculation by Keith Butler (personal communication) using the Opacity Project suite of programs. Again, note that the resonance structure is accounted for. As an example see Fig. 2, which shows the ground-state photoionization cross-section of Ti II.

Where accurate data were unavailable simple approximations were used which should generally be correct to within an order of magnitude.

The spectra of A supergiants are riddled with lines from iron-group elements and it is necessary to include them all in the line-formation calculations as a source of background opacity. Since we have the accurate photoionization cross-sections we need a method to include the background opacities which does not change the wavelength dependency, i.e., an opacity-sampling method. The basic concept applied is similar to the approach first introduced by Anderson (1989). The database is the full Kurucz (1988) line list. The energy levels are packed together into 'superlevels' – a single superlevel contains only levels of one

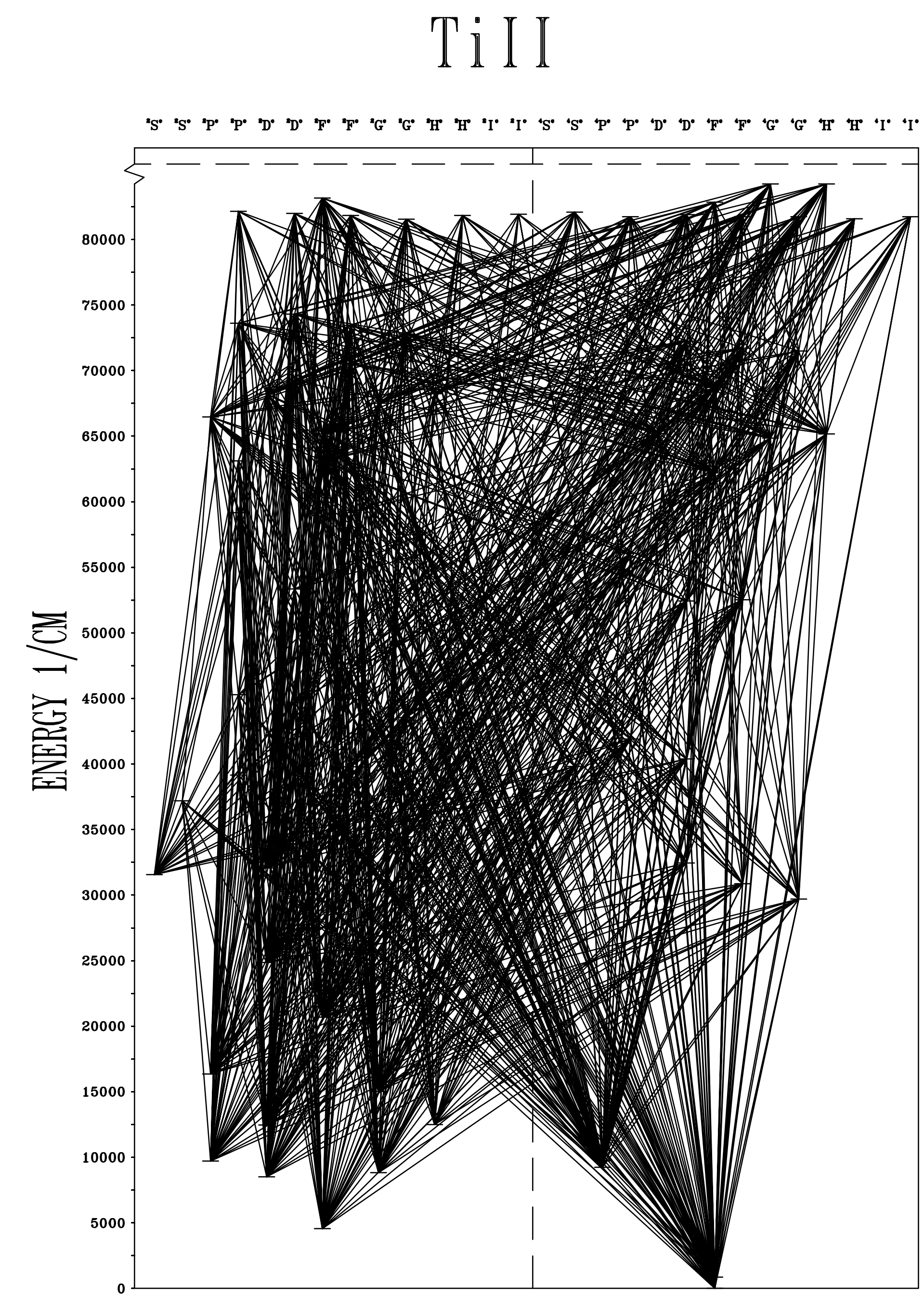


Figure 1. Grotrian diagram for Ti II

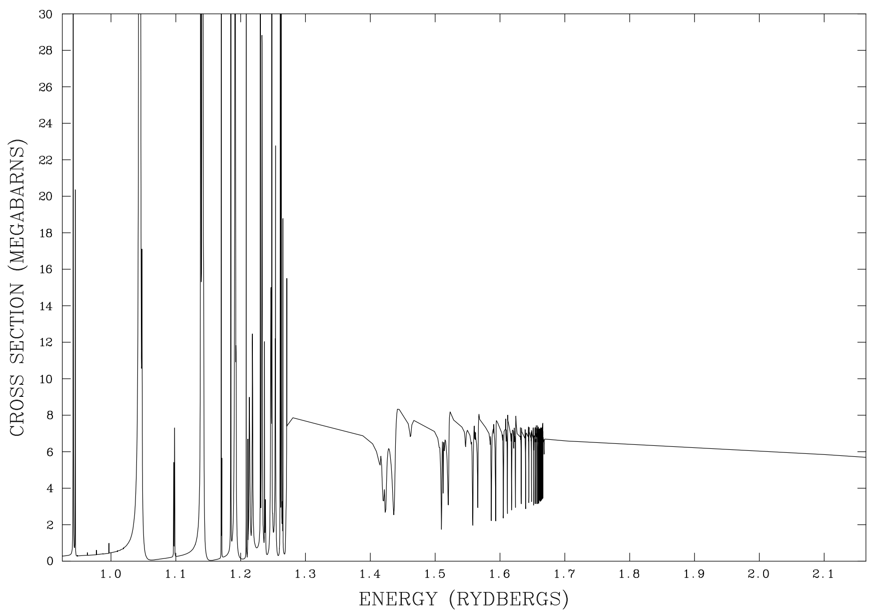


Figure 2. Photoionization cross-section for the ground state of Ti II. The entire resonance structure is included in our calculations.

parity – and are connected via 'supertransitions', i.e., highly complicated profile functions which can be tabulated. Figures 3 and 4 show two examples. The entire background model contains more than two hundred such cross-sections.

The advantage of this method is that it can easily be extended to treat the background opacities in non-LTE, which will be one of the next steps in our work. It is absolutely essential to take the background opacities into account because the non-LTE line formation would otherwise severely overestimate the ionizing continuum flux, leading to physically meaningless results (and numerical instabilities).

### 2.2. The Line-Formation Calculations

The programs used for the work presented here are DETAIL and SURFACE, which were written and first described by Giddings (1981). In the meantime, they have been modified significantly (K. Butler, personal communication) and now offer the ALI method (see the review by Hubeny 1992 for a description) as a solution scheme, as well as the original Rybiki-type scheme of Auer & Heasley (1976). The ALI operator as described by Puls (1991) is also included as an option so that the effects of mass loss can be studied in the comoving frame. Note that DETAIL/SURFACE is purely a line-formation package; i.e., the density stratification of the model atmosphere is not changed. Also, these programs are still in plane-parallel geometry, so lines formed far out in the wind cannot be reproduced correctly. However, it is to be expected that the lines we are inter-

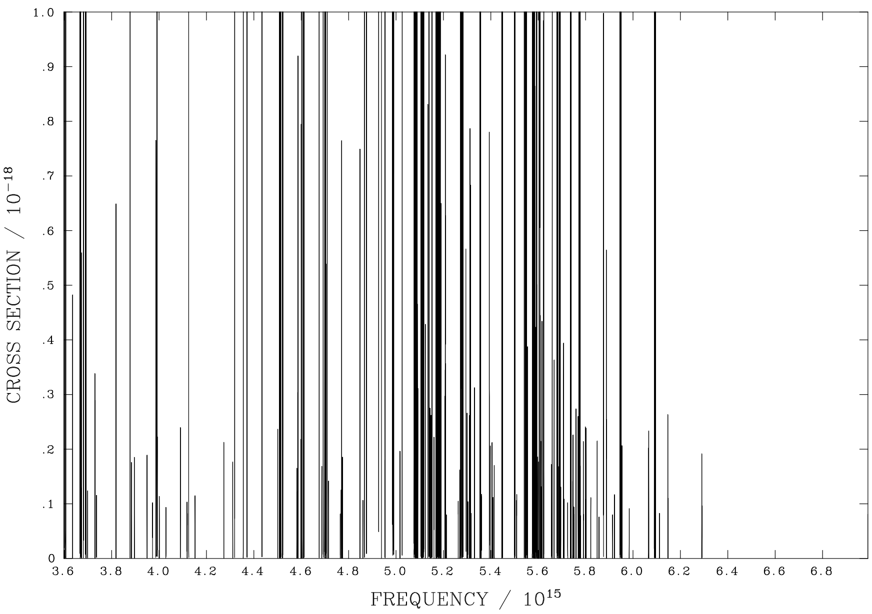


Figure 3. Sample of a 'supertransition' from the first even-parity to the third odd-parity superlevel in Fe II.

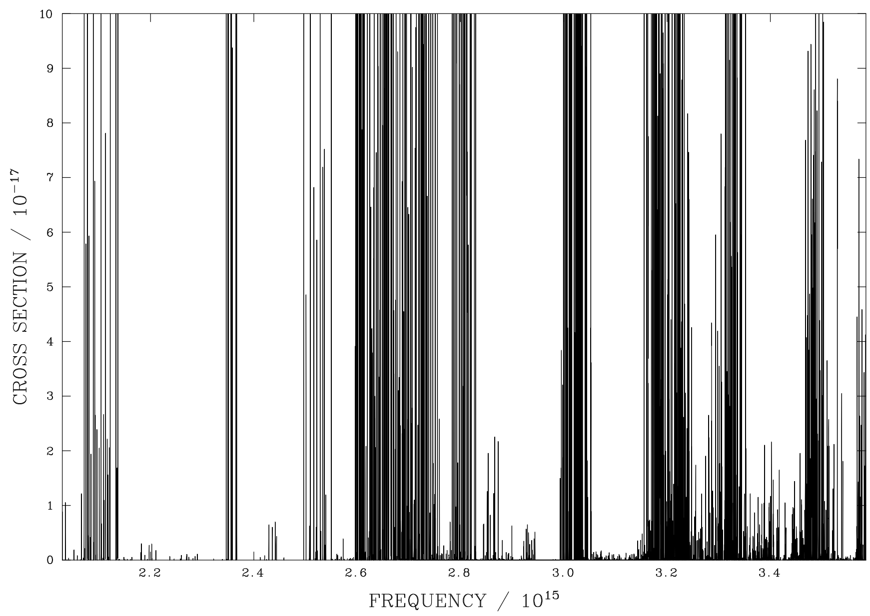


Figure 4. Sample of a 'supertransition' from the second even-parity to the second odd-parity superlevel in Fe II.

ested in will be mostly pseudophotospheric and should be adequately described using our approach.

## 3. First Results

The model atom for Fe II has been tested for the main-sequence A star Vega and for the moderately extended star $\eta$ Leo (A0 Ib). In both cases the results were promising, so we can put our trust in the non-LTE model atom in its current state. For reasons of brevity we will only show results for a more extreme object in this paper.

Similar tests have yet to be performed for Ti II. Thus, we do not regard our results to be as reliable yet as those for Fe II. More tests are needed and are under way.

We chose the star 41-3712 in M31 (A3 Ia-0) to test our models close to the Eddington limit where mass-loss effects are expected to be most significant. The spectrum was obtained with the Keck HIRES spectrograph by Jim McCarthy (more information can be found in Jim McCarthy's contribution to these conference proceedings; McCarthy et al. 1998). First LTE analyses show the object to have roughly solar abundances (McCarthy et al. 1997). The use of Kurucz ATLAS9 line-blanketed model atmospheres gives a fit to the observations at a temperature of 8400 K and log $g = 0.9$. The wind parameters have been derived using a SPH-type model atmosphere (Santolaya-Rey et al. 1997; see also Puls et al. 1998) at a slightly higher temperature to account for the lack of line blocking in the non-LTE model consisting of only hydrogen. The wind parameters are: $\dot{M} = 0.9 \times 10^{-6} M_{\odot}\mathrm{yr}^{-1}$, $R_{*} = 266 R_{\odot}$, and $v_{\infty} = 200 \mathrm{km\,s}^{-1}$. The structure of this model has been used in our line-formation calculations, rather than the hydrostatic ATLAS9 model. Figures 5 and 6 show the comparison of the theoretical lines with the observations for some randomly chosen lines of Fe II and Ti II, respectively. The theoretical lines are, in each case, LTE without, and non-LTE with, the velocity field. Actually, there is no difference between non-LTE with and without the velocity field for these lines since they are formed deep down in the atmosphere where the outflow velocities are unimportant.

As can be seen, the non-LTE effects for Fe II are small, whereas Ti II shows strong effects. Note that no fine tuning of the abundances has been made as yet; these results are based on solar-abundance calculations and are the first step of a detailed investigation. Ti II is temperature sensitive in the parameter regime that we are working in. Thus some work is required to determine the optimum parameters for the non-LTE model atmosphere used before an abundance analysis for this ion can be performed reliably. Figure 7 shows another part of the spectrum. The lines of Fe II and Ti II are reproduced well by the calculations. Note that the stronger Ti lines show smaller non-LTE effects than the weakest ones, and that the LTE values differ less from the observations than in the case of weaker lines.

Finally, Figure 8 contains one of the strongest Fe II lines in the observed spectral range. As is obvious from the shape of the profile, this line is affected by the stellar wind. The two theoretical profiles are LTE and LTE with the velocity field in the calculation. Obviously, our description suffices to calculate

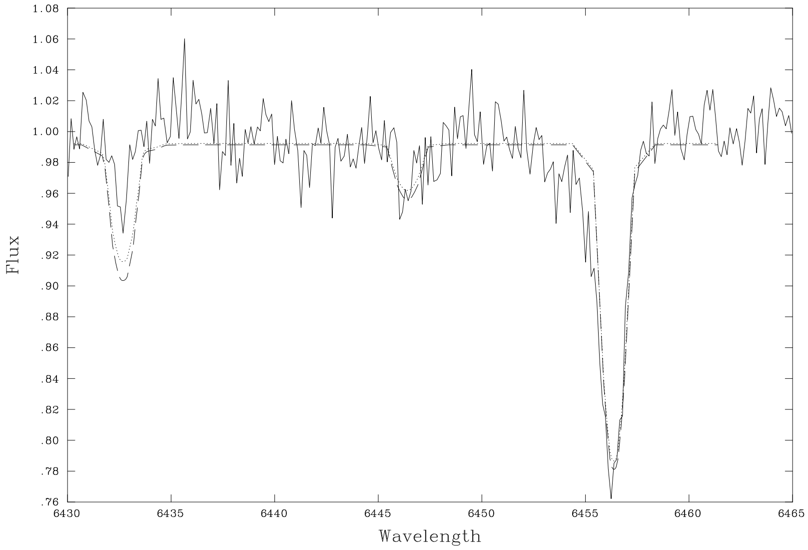


Figure 5. Part of the spectrum of 41-3712 showing lines of Fe II. Dashed line, LTE calculation; dotted line, non-LTE calculation allowing for the velocity field.

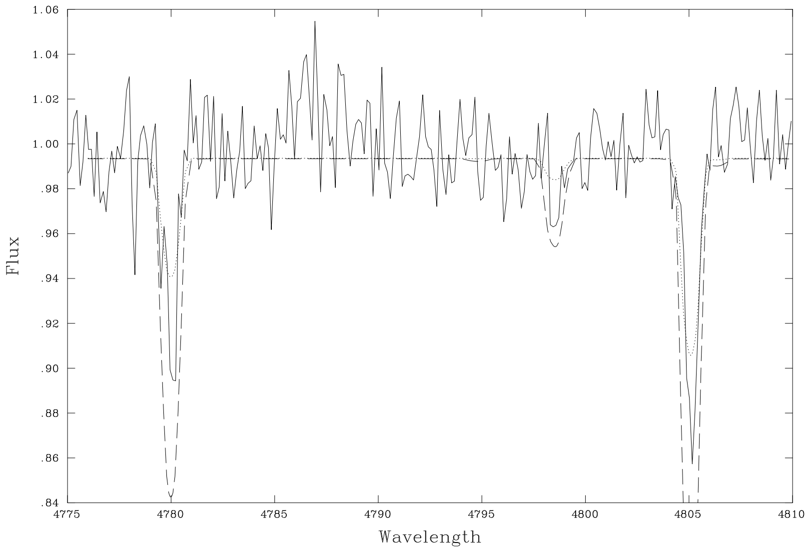


Figure 6. Part of the spectrum of 41-3712 showing lines of Ti II. Dashed line, LTE calculation; dotted line, non-LTE calculation allowing for the velocity field.

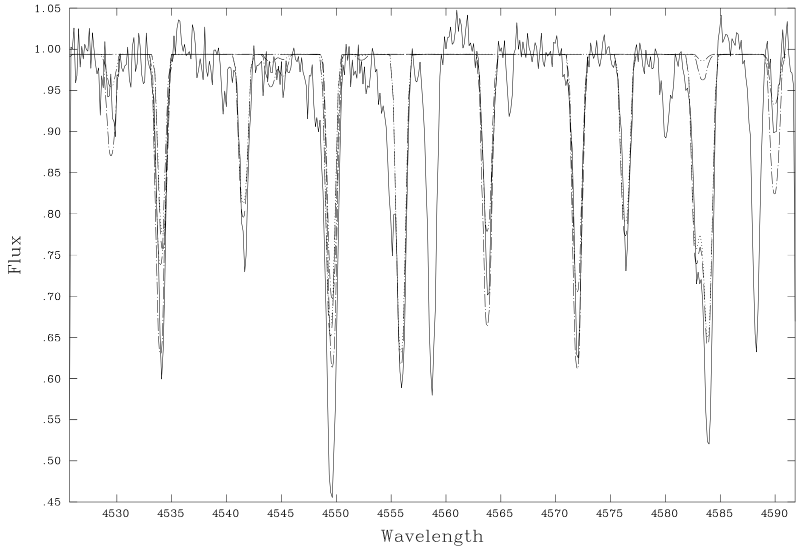


Figure 7. Part of the spectrum of 41-3712 showing lines of both Fe II and Ti II. Dashed line, LTE calculation for Fe; dotted line, non-LTE calculation for Fe allowing for the velocity field; dash-dot line, LTE calculation for Ti; dash-dot-dot line, non-LTE calculation for Ti allowing for the velocity field.

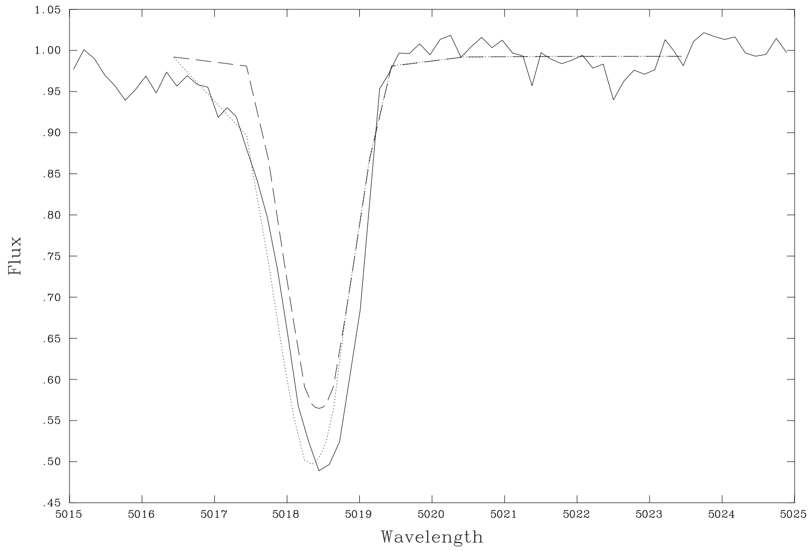


Figure 8. Part of the spectrum of 41-3712 showing one of the strongest lines of Fe II. Dashed line, hydrostatic LTE calculation; dotted line, LTE calculation allowing for the velocity field.

such lines reliably. Our approach will enable us to use the strong lines in the analyses of more distant stars even when they show wind contamination.

## 4. Summary and Outlook

We have developed model atoms for Fe II and Ti II for the analysis of non-LTE spectra of A supergiants. Fe II provides reliable results while Ti II needs to undergo further testing before it can be used routinely in analyses. Based on these models we can reproduce lines which form in the photosphere and in the lower parts of the wind. Sphericity effects seem to be still unimportant, even though the line centres of the strongest lines are formed as far out as seven stellar radii. The line-formation package DETAIL/SURFACE in its current form, together with the model atoms, can be used to analyze A supergiants without the restrictions which apply when limiting oneself to LTE and the hydrostatic approach; i.e., the stronger lines can be included in an analysis. Obviously, this approach will fail for lines like H$\alpha$, and in this case the full unified treatment as described by Santolaya-Rey et al. (1997) is required.

The work presented here prepares the stage for a multitude of projects which can now be tackled. We will soon be able to include the background opacities in non-LTE (this step may not be so important for the A supergiants but once understood we can also use such models for hotter stars). This approach will be used in an attempt to include line blocking in the SPH code. The findings of Pauldrach et al. (1998), as reported at this conference, will help to describe the effects of the wind in this case. It should be mentioned that the SPH code uses DETAIL input datasets (cf. Puls et al. 1998), so that the DETAIL model atoms can be easily transferred to the fully spherical case without problem, allowing lines showing stronger wind effects to be treated.

As has been outlined in the introduction, we will also attempt to produce a set of reliable strong lines to be used in the more distant objects and an assessment of the accuracies that can be achieved in analyses based on these lines. Further model atoms such as Cr II and perhaps others will be developed if they prove important.

All these individual projects will, in the end, provide the tools to understand A-supergiant atmospheres, to use A supergiants as reliable metallicity indicators, and thus to provide information needed for the understanding of the evolution of galaxies and to derive reliable distances using the WLR (Puls et al. 1996).

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## Discussion

**Puls:** When I see the beautiful results which Ivan [Hubeny] has presented, I ask myself – since I have to code all this at some time [laughter] – what is the advantage of your very detailed input with respect to his ‘packing’ of the levels? He also had very nice results in respect of the profiles [p. 108].

**Becker:** I think he uses the packed levels for his structure calculations, and he needs the full data for his spectral synthesis..? [Turning to Hubeny.]

**Hubeny:** No, the nice point is that there’s no difference between structure and line formation; everything’s done together. The reason I have to use ODFs is that, even with ODFs, there are already 18 000 frequency points.

**Puls:** But in non-LTE you had 30 levels or so, isn’t that right? The inversion of 30 levels is much easier than the inversion of 800 levels!

**Becker** [showing impenetrably dense Grotrian diagram]: It will be possible to pack these levels – in fact I have the packed levels – but for the line-formation step, in DETAIL as it is, I have to be a bit more careful how I go about it.
**Puls:** But apart from this, you see no advantages in using the full data?
**Becker:** Not necessarily.
**Hubeny:** The general question is not so much should you pack levels – there has always been some sort of packing; even in C IV you always pack fine-structure levels anyway, so it's not something new – but how you treat individual lines. Opacity *sampling* is a bit tricky because the doppler width is so small, and unless you had a very large turbulent velocity you'd have to use something like 0.01Å resolution instead of 0.1Å.

I'd also like to ask, do you think titanium might be important for the structure? Why did you choose Ti II?
**Becker:** Because when I'd modelled all the Fe II lines in my spectra, everything that was left was Ti II! And Fe I, which is the other important spectrum to look at, is more or less done.
**Prinja:** How did you constrain the velocity fields?
**Becker:** At the moment, the velocity-field structure is an input, provided by Achim's models.
**Kudritzki:** It's possible to analyse the H$\alpha$ profile for this. Particularly for the A supergiants which have well-pronounced P-Cygni profiles, you can get information about both $v_\infty$ and the $\beta$ index.