Including Mg I IR (<72000 Å) lines in solar and stellar models

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Abstract

Considering the imminent launch of the James Webb Space Telescope with IR spectroscopy capabilities, our ability of calculating reliable synthetic stellar spectra in this spectral range must be improved. An important species with strong features in the spectra of late-type stars is the neutral Mg. In the present work we have improved our previous Mg I atomic model by adding 128 strong transitions (log(g f)>−1), up to 72000 Å, and updated several atomic parameters. The energy levels for terms transitions were increased from 26 to 85 (3s.20p ^{1}P). One of the most important changes is our innovative treatment of the Effective Collision Strengths (ECS) parameters, which describes excitation by collision with electrons. We employed the latest R-matrix (RM) computations by Barklem et al. (2017)[1] up to level 25 (3s.6p ^{1}P). For transitions involving levels between 26 and 54 (3s.7i ^{1}I) we tested the influence in the spectrum of two different sets of ECS parameters: the widely used combination of Seaton [2] (allowed transitions) (SEA) plus van Regemorter [3] (forbidden transitions) (VRM) formulas, and our new ECS data obtained in this work using the multi–configuration Breit–Pauli distorted–wave (DW) method. For transitions to levels higher than 54 we completed the ECS with SEA+VRM data.

Method

We built three variants of the solar atmospheric model "1401" (Figure 1 and Table 1), which represents the dominant feature on the solar disk at magnetic minimum [4]. Each variant has a different Mg I atomic model:

- **1401a**. 26 levels. An update of the transition parameters, namely: oscillator strengths (gf), Einstein coefficients (A) [5]; and broadening data (Radiative, Stark and Van der Waals) [6,7]. The ECS from SEA+VRM was re-computed with the updated transition data.

- **1401b** and **1401c**. 85 levels (up to 3s.20p ^{1}P) to reproduce IR. Higher levels (55 to 85) were added as super-levels to include the exchange processes between Mg I and Mg II. Same updates than 1401a. The amount of levels for Mg II was also increased from 14 to 47 (up to 2p6.11g ^{2}G). Photoionization parameters was updated [8]. From 1 to 25 level (3s.6p ^{1}P) the available RM [1] ECS data was used in both models. **Most important differences between these models are the ECS for transitions involving levels 26 to 54 (3s.7i ^{1}I):**
  - **1401b:** ECS using SEA+VRM data
  - **1401c: new ECS data calculated by us with the multi–configuration Breit–Pauli distorted–wave (DW) method, using the AUTOESTRUCTURE code.**

  For transitions involving levels from 55 onward the ECS data was complemented with SEA+VRM.

The NLTE calculation and synthetic spectra for each model were computed using the SSRMP system.

The Solar Stellar Radiation Physical Modeling (SSRPM) system [3]

- Solves simultaneously transport and statistical equilibrium equations
- 1D plane-parallel atmosphere
- Populations of H, H-, H2 and 52 atomic species (neutrals and the next 2 ionization states) in full non-LTE with PRD
- Computes 198 species in higher ionization states using the nlte optically thin approximation
- 436977 spectral lines are computed for atoms and ions
- 2219276 diatomic molecular lines are computed in LTE

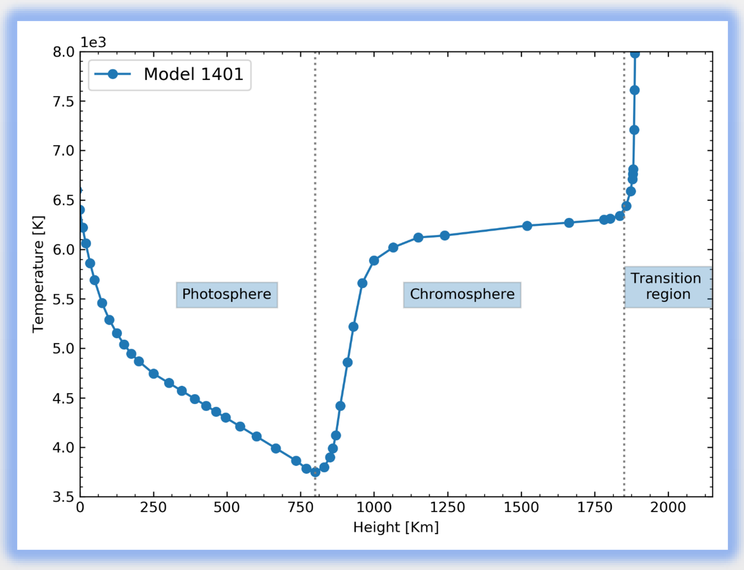


Figure 1. Atmospheric model 1401 [4]

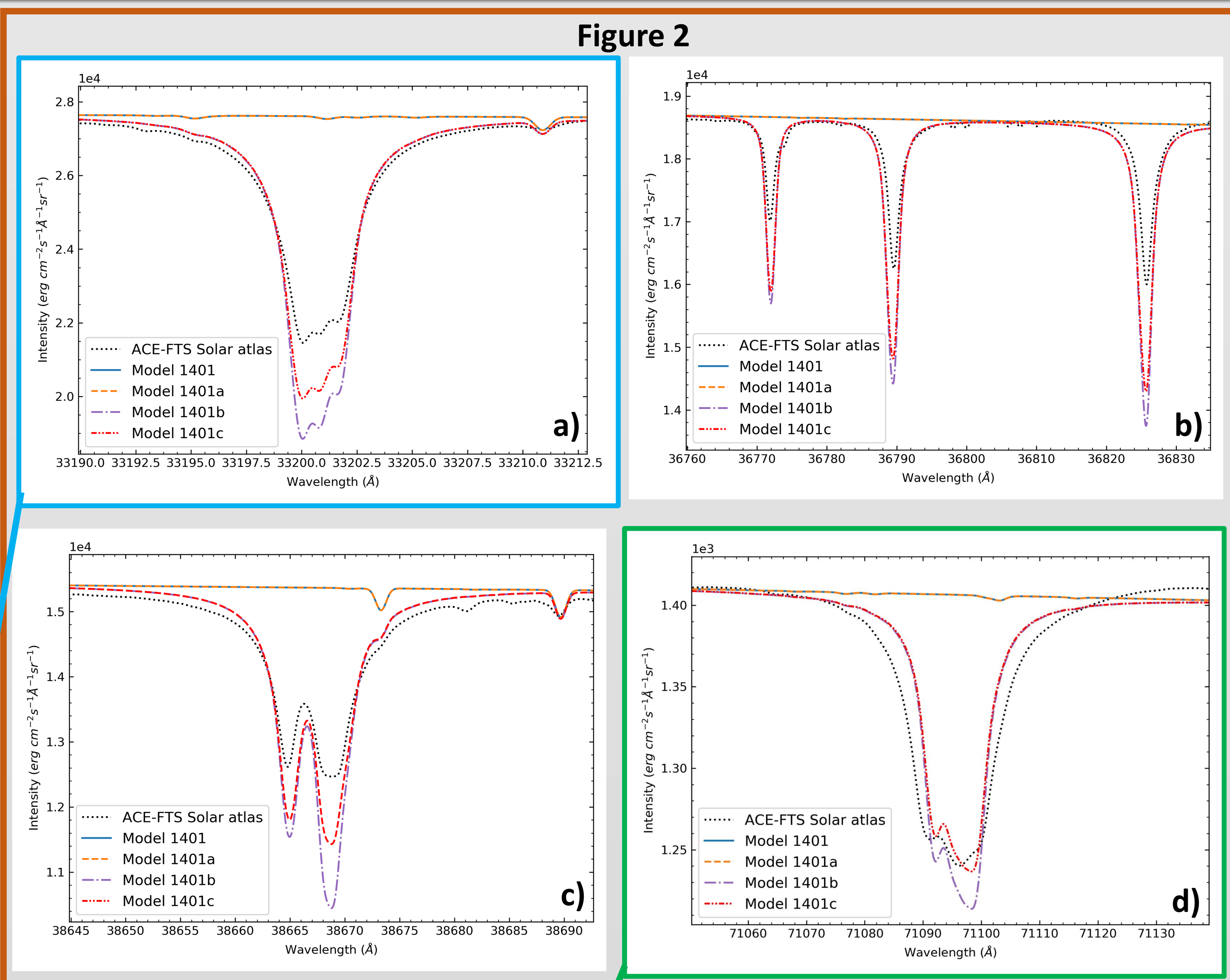
Model	Mg I levs	Mg II levs	ECS data (Mg I)	Notes
1401	26	14	SEA&VRM	Original model, Fontenla et al. (2015)
1401a	26	14	SEA&VRM	gf and broad. data updated
1401b	85	47	RM (< lev 26) + SEA&VRM (levs 26 to 85)	gf, broad. and photoioniz. data updated
1401c	85	47	RM (< lev 26) + DW (levs 26 to 54) + SEA&VRM (levs 55 to 85)	gf, broad. and photoioniz. data updated

Table 1. Models summary.

Results

Figures 2a-d show the calculated spectral lines compared with IR observations from ACE-FTS Solar Atlas [9]. Spectral features shown in panel a, c and d are the result of adding several unresolved transitions. All examples are new calculations, i.e. transitions that were not included in the original atomic model of Mg I with 26 levels. Models **1401** (blue solid-line) and **1401a** (orange dashed-line) show no line, and the spectra follows the continuum. On the other hand, models **1401b** (purple dash-dot line) and **1401c** (red dash-dot-dot-line) show an acceptable match with observations. **Although both models 1401b and 1401c produce deeper spectral lines than observed, model 1401c improves the match for all the studied lines.**

Figure 2



The depth of a spectral line is related to the difference in the population between the two levels involved at the formation region. In order to visualize how different the population of Mg I is re-distributed among levels in each model, Figure 3 shows the model population ratio (1401c/1401b) for each level, at the average formation height (250 Km, as an example). It can be seen that model 1401c has up to ~7% more Mg I in higher levels, due to the DW ECS that are always higher than SEA+VRM (at the formation temperature). DW ECS link high levels with lower levels (<25) using higher transition rates.

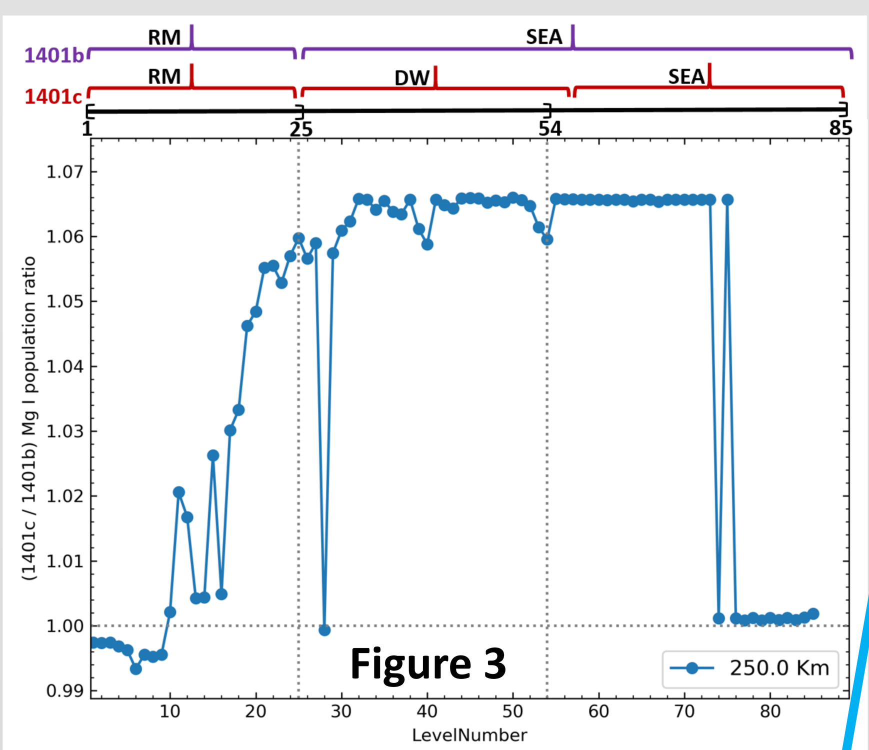


Figure 3

- **Line: 33200.647 Å** – Transition: 3s.4d ^{3}D (#13) - 3s.5f 3F (#24)

Transition using R-matrix ECS in both models, "Indirect change"

The contribution function (Figure 4a) for transitions that form the absorption feature in Figure 2a, shows that the formation region is approximately between 150 and 347 Km, in the photosphere (see Figure 1). In this points the population of level 13 is almost the same for both models (Figure 3), but the population of level 24 is higher in 1401c. This evidence the coupling between atomic levels: using different ECS in higher levels, **although the same ECS is used in this transition, DW ECS produces a redistribution of Mg I population among all energy levels, causing relevant changes in the spectrum.**

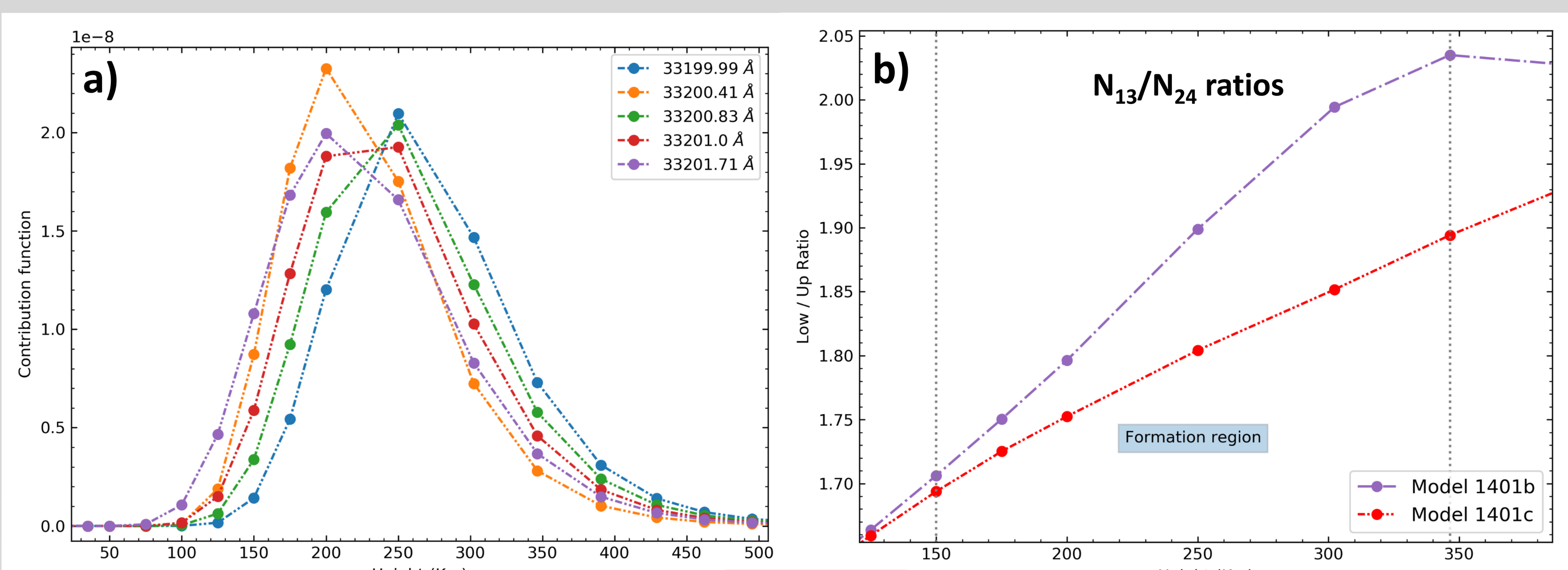


Figure 4

- **Lines: 71092 Å** - Transition 3s.5f ^{1}F (#23) - 3s.6g ^{1}G (#37) and **71097 Å** - Transition 3s.5f ^{3}F (#24) - 3s.6g ^{3}G (#38)

Transition using SEA (1401b) vs DW (1401c) ECS data, "Direct change"

As an example for line 71097 Å, Figure 5a shows almost a factor 3 between the DW (red dash-dot-dot line) and SEA (purple dash-dot line) collisional data. Figure 5b shows how this difference in the ECS for the involved levels produces a direct change in the levels population, combined with indirect changes from the other levels.

Figures 4b and 5b shows the 1401b and 1401c *levels population ratio* (N_{low}/N_{up}) variation vs height for the lines in Figures 2a and 2d, respectively. It can be seen that **the ratios for model 1401b are larger than for 1401c, which is coherent with shallower lines in the synthetic spectra of the model 1401c, as we have seen in the majority of the spectral features across the IR range, improving the match with observations.**

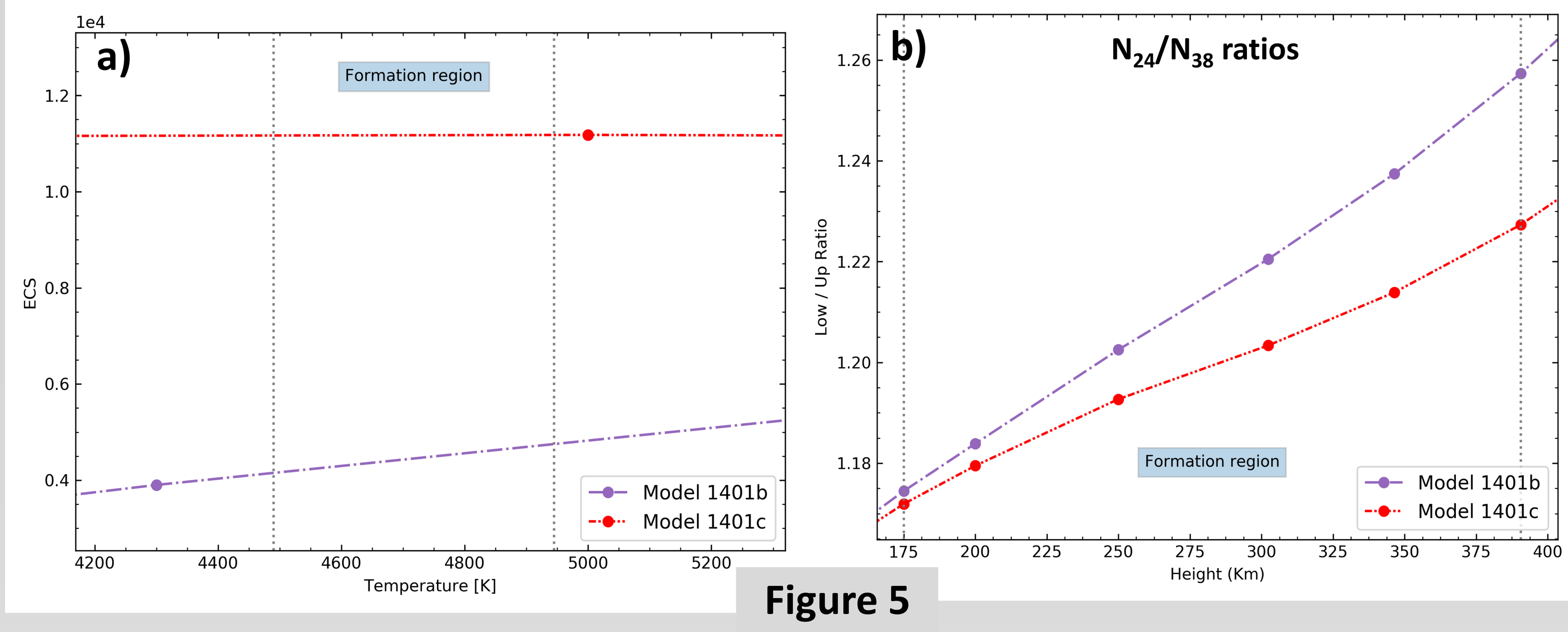


Figure 5

Current conclusions

We found an overall better agreement between observed and synthetic IR spectral lines, when the combination R-matrix and our Distorted Wave calculation for the collision with electrons data (ECS) were used in higher levels (model 1401c). This result opens the possibility of a new and more reliable approach than the widely used formulas of Seaton and van Regemorter, as methods of calculating ECS for Mg I and other species in stellar atmospheres, when the R-matrix method is not available.

References

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