ACCURATE SPECTROSCOPY OF INTERMEDIATE AND LATE SPECTRAL TYPES

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ABSTRACT. Elemental abundances in the Sun and in meteorites are examined with respect to their qualification as a standard of population I composition. Some problems that arise in connection with spectroscopic determinations of abundances in the Sun, and in other late-type stars, are discussed with emphasis on photospheric models and departures from LTE.

1. SOLAR AND METEORITIC ABUNDANCES

We are in the fortunate position of having solar matter in condensed form at our disposal which can be subjected to extremely accurate analysis. That there is indeed some type of meteoritic matter whose chemical composition closely matches that of the Sun is by no means trivial, yet it is by now well-established that carbonaceous chondrites contain elements with very different cosmochemical properties in solar proportions. The present situation is illustrated in Fig. 1, which shows elements whose solar abundances are believed to be accurate to within about ± 50 percent, as judged from available spectral lines and f-values. A closer comparison, at the ± 20 percent level, has been accomplished for six elements with favourable spectroscopic properties (Holweger 1979). As it turned out, the abundance ratios in the Sun agreed with those in Cl chondrites in all cases. No other type of meteorite was found to fit the solar composition so closely.

This close relationship between solar and meteoritic matter does not preclude that solar-system matter as a whole has suffered chemical fractionation on the long way from the sites of nucleosynthesis into the solar nebula. A sensitive test for cosmochemical fractionation was devised by Suess (1947). He noticed that the abundance of odd-mass nuclides belonging to elements of different volatility and geochemical type tended to be a smooth function of mass number, reflecting nuclear rather than chemical processes. Anders and Ebihara (1982), repeating the test with modern abundance data, confirmed this smoothness. Any significant cosmochemical fractionation - exceeding 15% or so - would

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have appeared as perceptible irregularities in the abundance curve.

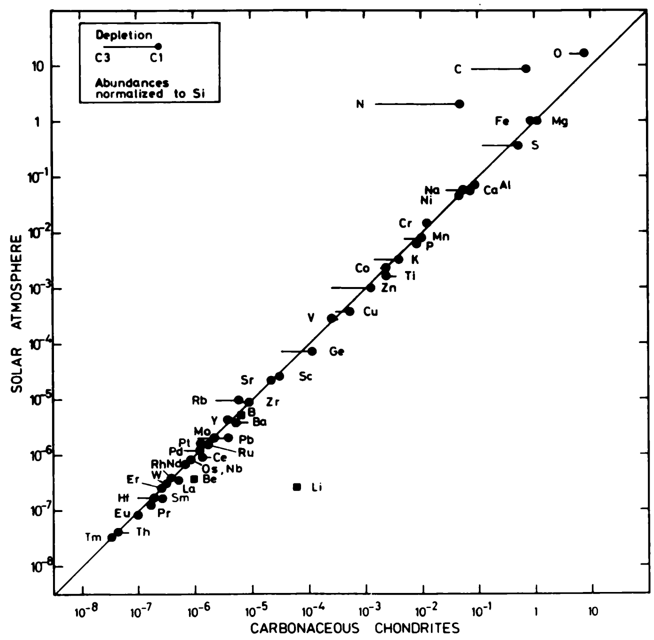

Figure 1: Comparison of solar and meteoritic abundances (carbonaceous chondrites of type 1 and 3).

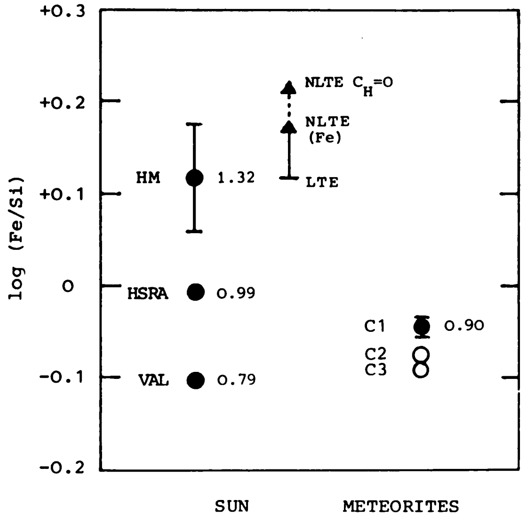

Figure 2: The Fe/Si ratio in the Sun and in carbonaceous chondrites of types 1, 2 and 3.
Solar abundances (HM model): log N(Fe) = 7.673 ± 0.017 (Blackwell et al. 1984); log N(Si) = 7.55 ± 0.05 (Becker et al. 1980). Meteorites: Anders and Ebihara (1982, C1 chondrites), Mason (1971, C2 and C3). For further details see text.

Thus, the elemental (and isotopic) composition of C1 chondrites may be assumed to be typical for the condensable fraction of population I matter. Surprisingly enough, the Sun may be slightly non-standard. If we compare the solar and meteoritic ratio of the two key elements representing the siderophile and lithophile geochemical groups - iron and silicon - then a puzzling discrepancy appears (Fig. 2): the solar ratio Fe/Si = 1.32 is well above the value of 0.90 found in Cl chondrites. This poses a number of questions.

Taken at face value, this result is not implausible as soon as we view the Sun and meteorites as parts of the inner and outer solar system. It is well known that the global Fe/Si ratios of the terrestrial planets - the fractional mass of their iron core - increase towards the Sun. So the Sun itself would conform to this trend. We must bear in mind the possibility of a Fe/Si fractionation in the early solar system. Such processes might also have affected other stars and may contribute to the spread of Fe/Si ratios observed among population I F- and G-type dwarfs (Andersen et al., this conference). Gustafsson (this conference) noticed that the mean Fe/Si ratio in this sample is below the solar value, closer to that found in Cl chondrites.

However, we must also consider the possibility that the disagreement between the solar and meteoritic Fe/Si ratio is fictitious and due to our imperfect understanding of photospheric structure and spectrum line formation. This will be discussed in the next section.

2. MODELLING THE ATMOSPHERES OF SOLAR-TYPE STARS

2.1. One-Component Solar Models

The error bar quoted in Fig. 2 is the standard deviation of abundance values derived from individual lines and does not include any systematic error. The iron abundance is based on low-excitation Fe I lines (E.P. = 0-2.6 eV), whereas the Si lines are of the high-excitation type (4.9-6.0 eV). Thus, the inferred Fe/Si ratio is quite sensitive to errors in the temperature structure of the photospheric model employed.

This model-dependence is illustrated in Fig. 2. The value of 1.32 for Fe/Si, discussed in the previous section, was obtained using the HM model (Holweger and Müller 1974). If the same set of lines is analysed using the HSRA (Gingerich et al. 1971) or the VAL model (Vernazza et al. 1976), considerably lower Fe/Si values result, the logarithmic difference VAL minus HM amounting to -0.22 dex. The situation would be much more satisfactory if accurate f-values for high-excitation Fe I lines, or Fe II lines, were available: the model dependence, VAL-HM, would then reduce to -0.07 dex for 4.5 eV Fe I lines, and to +0.04 dex for 2.8 eV Fe II lines, respectively.

Deviations from LTE constitute another problem, though probably a less serious one. Recent NLTE studies (section 3.2) lead to abundance corrections of about 0.06 dex for low-excitation lines of Fe I (Fig. 2). This value would increase to 0.1 dex if neutral-atom collisions were neglected (denoted by '$C_H = 0$' in Fig. 2). No data are available for Si I . If the NLTE corrections are similar then the effect on the ratio of both elements will be smaller than indicated in Fig. 2.

How good are the *solar models*? It is tempting to remove the Fe/Si problem by simply choosing the VAL model as the appropriate one. However, there is a more realistic, more sensitive test for solar models than the comparison of solar and meteoritic abundances: to compare solar abundances derived from infrared molecular lines belonging to the same molecular band but differing in excitation potential. Vibration-rotation lines of OH and CO, and pure rotation lines of OH, have been studied in this way (Goldman et al. 1983, Grevesse et al. 1984, Sauval et al. 1984, Harris et al. 1987). The three main advantages of these lines are (i) high temperature sensitivity, (ii) likely to be found in LTE, (iii) very accurate relative f-values. In all cases, the HM model passed the examination but the other models did not.

At the same time the OH lines near 11 microns bring to light the limitations of *one-component model atmospheres*. All these models, including the HM, failed to reproduce the center-to-limb behaviour, at least close to the limb (Deming et al. 1984). The layers probed in this way are around $\tau_{5000} = 10^{-3}$. Deming et al. interpreted this as evidence for horizontal temperature inhomogeneities (thermal bifurcation) in the uppermost photosphere.

In view of this we will also have to investigate the effect of thermal inhomogeneities in the *lower photosphere*, associated with convective motions, on abundance determinations. While this is a task for the future, I wish to mention another problem that may occur in abundance determinations of solar-type stars. It is related to the *vertical* thermal structure of the photosphere.

2.2. Photospheric Abundances and Chromospheric Activity

It is well known that some G-type dwarfs possess chromospheres whose activity is much higher than that of the Sun. There is evidence that this "activity" is also perceptible in the photospheric line spectrum and may lead to fictitious underabundances if ignored. I have encountered this problem when analysing spectra of two dwarfs with very different chromospheric activity: 61 Vir (G6 V, quiet chromosphere) and Xi Boo A (very active chromosphere). The study was based on high-S/N spectra recorded with the ESO Coudé Echelle Spectrometer. The same set of 16 Fe I and 2 Fe II lines was used in both stars, giving greater weight to magnetically insensitive lines. Equivalent widths ranged from 7 to 245 mÅ. A model-atmosphere analysis was carried out using scaled solar models whose effective temperature and gravity were determined from colours and from the Fe I/II balance, respectively. The microturbulence parameter was adjusted such as to make abundances derived from medium strong and weak lines agree. The following parameters T_{eff}/log g/micro(km/s) resulted:

61 Vir: 5560/4.4/1.05; Xi Boo A: 5390/4.2/1.55.

In the case of *61 Vir*, the star with the inactive chromosphere, abundances derived from the various lines yield a highly consistent picture: weak and strong lines agree and the spread is quite small, attesting to the quality of the CES spectra. The iron abundance derived from the nine weakest and most Zeeman-insensitive lines is

[Fe/H] = +0.01 ± 0.02 (s.d.), i.e. perfectly solar.

The situation is quite different in the case of the active-chromosphere star Xi Boo A, although the spectra are of the same high quality and the analysis is done in exactly the same manner. Among the weaker lines, the scatter is twice as large and the iron abundance becomes [Fe/H] = -0.19 ± 0.04. This apparent underabundance is somewhat surprising in the case of an obviously quite young star. Much more disturbing is the fact that the three strongest lines (including one with Landé factor zero) lie about 0.2 dex above the weaker ones. Increasing log g from 4.2 to 4.55 will shift these pressure-sensitive lines downwards to match the weak ones, but then the Fe II lines will move upwards. To restore the ionisation equilibrium, T_{eff} has to be increased. If T_{eff} is treated as a free parameter, a scaled solar model characterised by 5690/4.8/1.05 meets both constraints set by Fe I/II and strong/weak lines. The iron abundance then becomes [Fe/H] = 0.00 ± 0.05. However, such a high effective temperature - 300 K hotter than derived from the colours - appears inacceptable. There is a simple way out of the dilemma: to restrict the temperature enhancement to the line-forming layers, thus keeping T_{eff} essentially unchanged. This also requires some iterative adjustment of log g, since the strong/weak line balance depends on the photospheric temperature gradient, and of T_{eff} in order to keep Fe I/II in balance. One possible model is characterised by a temperature enhancement of 200 K at optical depths smaller than 0.1, the other parameters being 5480/4.7/1.55. The iron abundance then becomes [Fe/H] = -0.03 ± 0.05, i.e. essentially solar.

Of course, this modified model of Xi Boo A is by no means uniquely defined but the trend is obvious: if excess photospheric heating is taken into account the underabundance tends to disappear.

Xi Boo A is not the only active late-type candidate of this kind. Cayrel et al. (1985) noticed anomalously low iron abundances in two Hyades dwarfs with high chromospheric activity. They suspected this to be due to chromospheric filling-in of photospheric lines. Another prominent object is ε Eri. Just like Xi Boo A, ε Eri is found to be metal deficient by 0.2 dex, when analysed with an unmodified scaled solar model (Steenbock and Holweger 1981). Indeed, in Fig. 1 of that paper, the strongest line is seen to deviate from the weaker ones as in Xi Boo A. There seems little doubt that the apparent underabundance of ε Eri disappears if excess photospheric heating is accounted for in the photospheric model. Interestingly, not only the thermal structure appears to be modified in these active stars but also the hydrodynamics: both exhibit anomalously high microturbulent velocities.

3. DEPARTURES FROM LTE IN STARS OF INTERMEDIATE AND LATE SPECTRAL TYPE

3.1. Observational Evidence

Departures from LTE that affect abundances were found by Ruland et al. (1980) in a detailed analysis of high-quality photographic spectra of the red giant Pollux (KO III). When LTE was assumed, a typical pattern of inconsistencies appeared among iron-group elements. Abundances derived from individual lines of low excitation potential were found to be lower than those obtained from high-excitation lines by 0.3-0.5 dex. This dichotomy was largest for lines on the flat portion of the curve-of-growth. Similar trends were observed by Brown et al. (1983) and by other authors in G and K giants in general. Steenbock (1983) and Magain (this conference) have found NLTE effects in halo giants.

In contrast to these low-gravity objects, main-sequence stars are expected to show less conspicuous departures from LTE. Abundance anomalies due to NLTE have been suspected in the AOV standard Vega (Gigas 1986, and references therein) and Procyon (F5 IV-V; Steffen 1985). In the Sun (G2 V), high-precision spectroscopy and f-values have made it possible to discern NLTE effects in Ti I and Cr I at the 10-20% level (Blackwell et al. 1987).

3.2. Statistical-Equilibrium Calculations for Cool Stars

Recent NLTE calculations have taken into account the thermalising effect of inelastic collisions with hydrogen atoms and made efforts towards a realistic representation of the atomic term structure and the ionising UV radiation field. Here, I would like to report some unpublished results for iron, obtained by W. Steenbock in Kiel, a continuation of earlier work (Steenbock and Holweger 1984, Steenbock 1985, Watanabe and Steenbock 1986). The Fe I/II/III model atom comprises 79+20+1 levels and 52+23 line transitions (see Gigas 1986). The results are expressed in terms of the NLTE abundance corrections $\Delta \log \epsilon$ to be added to the (logarithmic) abundances derived from observed equivalent widths of individual lines under the assumption of LTE.

Pollux. Fig. 3 shows the results for a typical red giant with T_{eff} = 4840 K, log g = 2.2, and solar metallicity such as appropriate for Pollux (KO III). Most $\Delta \log \epsilon$ values are positive, indicating a general overionisation of Fe I. When compared with the above-mentioned empirical results (see Fig. 4 in Ruland et al. 1980), an agreement is noted which gives some confidence in these fairly involved computations. In particular, the dependence of $\Delta \log \epsilon$ on excitation potential and line strength is reproduced. The relatively large NLTE corrections for lines of intermediate strength can be understood: these lines are almost box-shaped, with dark cores and practically no damping wings. Thus, their equivalent width is formed in the uppermost photosphere where departures from LTE are larger.

The thermalising effect of inelastic collisions with hydrogen atoms is important in Pollux. The $\Delta \log \epsilon$ values shown in Fig. 3 are derived by applying a scaling factor S_H = 0.2 to Drawin's approximation for the cross-sections, in accordance with Watanabe and Steenbock (1986). If we choose S_H = 1 instead, the calculated NLTE effects become too small. If we neglect neutral-atom collisions, on the other hand, the spread in the $\Delta \log \epsilon$ values increases from about 0.3 dex to 0.6 dex. Not shown in Fig. 3 are the NLTE corrections for Fe II lines, simply because they are so small (see also Steenbock 1985).

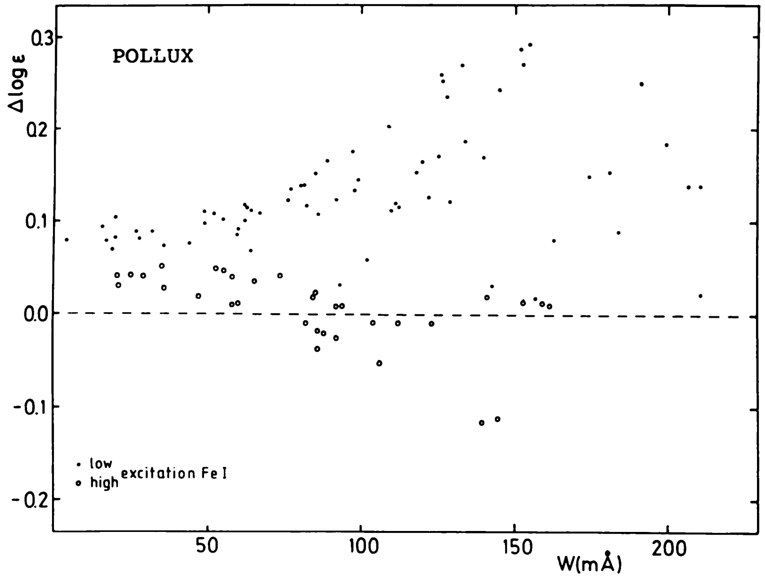

Figure 3: NLTE abundance corrections for Fe I lines in the red giant Pollux (KO III) (Steenbock 1987).

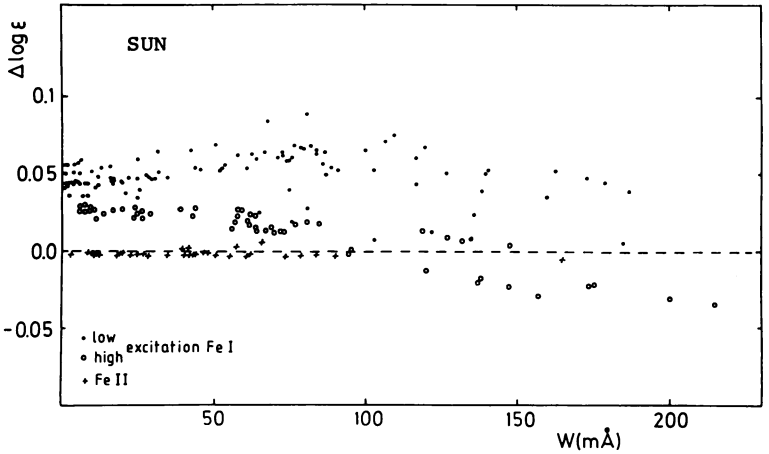

Figure 4: NLTE abundance corrections for the Sun (G2 V) (Steenbock 1987).

Arcturus (K2 III). Similar calculations have been performed for T_{eff} = 4260 K, log g = 0.9 and one-third solar metallicity. These parameters may represent a more evolved object than Pollux. The results are qualitatively similar. Surprisingly, despite the lower gravity, the NLTE corrections turned out to be a factor of two smaller than in

Pollux, at least for lines weaker than about 60 mÅ. This is probably due to the combined effect of reduced temperature and metallicity on the UV radiation field. Again, Fe II lines are in LTE.

Main-Sequence Stars. NLTE abundance corrections for the Sun (G2 V) are shown in Fig. 4. The pattern is similar to that of Pollux, but the NLTE effects are much smaller because of the increased frequency of collisions with hydrogen atoms and electrons. If the neutral-atom collisions were neglected, the $\Delta \log \epsilon$ values would increase by a factor of two. The results displayed in Fig. 4 are valid for the HM model. If the HSRA is used instead, somewhat larger departures from LTE result, but the overall pattern remains the same.

In the Sun, NLTE corrections for iron are small, amounting to at most 0.06 dex for low-excitation Fe I lines. The $\Delta \log \epsilon$ values for high-excitation lines are about half as large, while Fe II lines are in LTE. This weak sensitivity to NLTE effects is another attractive property of the latter two types of lines in addition to the weak model-dependence of their LTE abundances mentioned in section 2.1. Other iron-group elements in the Sun may be expected to exhibit similar departures from LTE. Indeed, NLTE effects of this magnitude are apparent in the high-precision LTE analysis of solar Ti I and Cr I by Blackwell et al. (1987).

Similar NLTE calculations have been carried out for two hotter main-sequence stars, Procyon (F5 IV-V) and Vega (A0 V). The results for Vega have reported elsewhere (Gigas 1986, and this conference). For Procyon, a flux-constant model with T_{eff} = 6500 K, log g = 4.0 and solar metallicity was adopted. The resulting pattern is quite similar to that in Fig. 4, with the important exception that the departures from LTE are significantly larger than in the Sun. The $\Delta \log \epsilon$ values for low-excitation Fe I lines weaker than 50 mÅ are typically 0.12 dex, while high-excitation lines deviate only by 0.07 dex, and Fe II is in LTE. Again, the largest departures occur in the equivalent width range 100-150 mÅ, with $\Delta \log \epsilon$ values of up to 0.20 dex.

3.3. NLTE and Galactic Chemical Evolution

The dependence of NLTE abundance corrections on effective temperature, gravity and metallicity will have to be studied in a more systematic manner, and for a variety of elements. Increasingly precise stellar spectra combined with differential model-atmosphere analyses permit the investigation of subtle abundance trends in galactic stellar samples which are important as constraints on models of galactic structure and evolution. Recent illustrations of the high accuracy that can be obtained are the studies of galactic disk stars by Tomkin et al. (1985) and by Nissen et al. (1985) with the supplementary data reported by Andersen et al. (this conference).

One of the basic assumptions made is LTE. This may be critical as soon as one deals with small abundance trends as a function of metallicity or, explicitly or implicitly, as a function of effective temperature or gravity. For example, one important subject of these studies is the possible variation of the abundance ratio (odd-Z elements)/Fe with Fe/H. The odd-Z elements are determined from lines of Na I and Al I, species whose ionisation potential is 5.1 and 6.0 eV, respectively - much lower than that of Fe I (7.9 eV). Thus, departures from LTE in the ionisation balance are likely to be larger for the odd-Z elements than for iron. Ignoring NLTE effects may introduce fictitious dependences of (odd-Z/Fe on Fe/H or T_{eff}. Real trends may be either exaggerated or underestimated in this way.

REFERENCES

Anders, E., Ebihara, M. 1982, Geochim. Cosmochim. Acta **46**, 2363.

Becker, U., Zimmermann, P., Holweger, H. 1980, Geochim. Cosmochim. Acta **44**, 2145.

Blackwell, D.E., Booth, A.J., Petford, A.D. 1984, A.A. **132**, 236.

Blackwell, D.E., Booth, A.J., Menon, S.L.R., Petford, A.D. 1987, A.A. **180**, 229.

Brown, J.A., Tomkin, J., Lambert, D.L. 1983, Ap.J. **265**, L93.

Cayrel, R., Cayrel de Strobel, G., Campbell, B. 1985, A.A. **146**, 249.

Deming, D., Hillman, J.J., Kostiuk, T., Mumma, M.J. 1984, Solar Phys. **94**, 57.

Gigas, D. 1986, A.A. **165**, 170.

Gingerich, O., Noyes, R.W., Kalkofen, W., Cuny, Y. 1971, Solar Phys. **18**, 347.

Goldman, A., Murcray, D.G., Lambert, D.L., Dominy, J.F. 1983, Mon.Not.R.astr.Soc. **203**, 767.

Grevesse, N., Sauval, A.J., Dishoeck, E.F. 1984, A.A. **141**, 10.

Harris, M.J., Lambert, D.L., Goldman, A. 1987, Mon.Not.R.astr.Soc. **224**, 237.

Holweger, H., Müller, E.A. 1974, Solar Phys. **39**, 19.

Holweger, H. 1979, XXIInd Liège Internat. Astrophys. Symposium, Université de Liège, p. 17

Mason, B. (Ed.) 1971, Handbook of Elemental Abundances in Meteorites, Gordon and Breach, New York.

Nissen, P.E., Edvardsson, B., Gustafsson, B. 1985, in Proc. ESO Workshop on Production and Distribution of C, N, O Elements, I.J. Danziger, F. Matteucci, K. Kjär (eds.), Garching, p. 131.

Ruland, F., Holweger, H., Griffin, R., Biehl, D. 1980, A.A. **92**, 70.

Sauval, A.J., Grevesse, N., Brault, J.W., Stokes, G.M., Zander, R. 1984, Ap.J. **282**, 330.

Steenbock, W., Holweger, H. 1981, A.A. **99**, 192.

Steenbock, W. 1983, A.A. **126**, 325.

Steenbock, W., Holweger, H. 1984, A.A. **130**, 319.

Steenbock, W. 1985, in Cool Stars with Excesses of Heavy Elements, M. Jaschek, P.C. Keenan (eds.), D. Reidel, p. 231.

Steenbock, W. 1987, private communication.

Steffen, M. 1985, A.A. Suppl. Ser. **59**, 403.

Suess, H.E. 1947, Z. Naturforsch. **2a**, 311.

Tomkin, J., Lambert, D.L., Balachandran, S. 1985, Ap.J. **290**, 289.

Vernazza, J.E., Avrett, E.H., Loeser, R. 1976, Ap.J. Suppl. **30**, 1.

Watanabe, T., Steenbock, W. 1986, A.A. **165**, 163.

DISCUSSION

BUDGE You showed graphs of abundance determinations for a chromospherically active dwarf using a conventional model and a model with a hot upper photosphere. It appears from these graphs that the abundances derived from weak lines were affected more by the hot upper photosphere than the abundances from the strong lines. Intuitively it seems to me that the weak lines would be less affected than the strong lines.

HOLWEGER Weak lines are not necessarily formed in deeper layers. For example, weak molecular lines, or Li I 6708, are formed in the upper photosphere.

The evidence for a hot upper photosphere of Xi Boo A is indirect. When using a scaled solar model, abundances derived from strong and weak lines are found to disagree. This cannot be removed by changing the upper photospheric temperature because the height of formation of strong and weak lines is not sufficiently different. It can be removed by an increase of gravity, i.e. pressure broadening. This also affects the ionization balance, which can be restored by making the line-forming layers hotter.

RUTTEN I have two comments. First, it is important to realize that most high-excitation lines observed in optical spectra are also most probably lines with log gf > -2. They provide the most probable depopulation path for all levels at about their upper-level excitation energy, and their departure coefficients drop below unity where the lines start feeling the surface. This excitation deficiency affects their source function, and may cancel the effect of collective overionization, which reduces the populations and opacities but not the source functions. So, a difference between low and high excitation lines can result from this cancelling effect : two NLTE mechanisms are acting together and making high-excitation lines appear seemingly in LTE.

My second comment is on the standard solar models. You don't have to compare the HOLMUL model any more with the HSRA or VAL models. These latter models represent a progression in the sophisticated NLTE solar continuum modeling at Harvard that has now culminated in a model of which the photospheric part is nearly the same as HOLMUL, and in which the metal overionizations in the temperature minimum region are much smaller than for the older, cooler models. Simply because the flatter gradient keeps B_ν closer to J_ν in the ultraviolet. This came about because Avrett now includes more of Kurucz's ultraviolet line list in detail, so shifting the computed height of formation of the observed continua outward, and flattening the temperature gradient.

I should add here that even though these models possess chromospheres in contrast to HOLMUL, the actual model assumed for the ultraviolet line haze within the fitting procedure is without one. Avrett specifies line source functions for the haze lines that are set to scattering near the temperature minimum in an ad-hoc parametrization, effectively adopting the HOLMUL model as a line excitation temperature. So, although the HOLMUL model is never mentioned in the Harvard work, it has in effect been retrieved and verified by it -within the constraints of plane-parallel modeling.