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The Determination of the Solar Iron Abundance from Fe I Lines

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Abstract. We revise the solar photospheric abundance of iron derived from Fe I lines using two similar scales of oscillator strengths, the precise Oxford scale of Blackwell et al. and the new scale of Bard et al. To explain a puzzling discrepancy between the resulting abundances of Holweger et al. based on the latter scale and the earlier Oxford one we analyse sources of errors in the solar iron abundance determinations. The most important reason for the discrepancy is connected with the damping enhancement factor, E. The anomalous behavior of Fe I ~ 2.2 eV lines noted by Blackwell et al. is also discussed. The abundance anomaly is primarily due to uncertainties of observed equivalent widths and is statistically insignificant. However, whether the photospheric iron abundance is less than the meteoritic value remains unsettled.

1. Introduction

The solar iron abundance has been much discussed in the literature. The determinations by Holweger et al. (1990) and Biemont et al. (1991) based on the analyses of Fe II lines lead to a "low" abundance value between $A_{Fe} = 7.48 \pm 0.09$ (on the logarithmic scale where $\log A_H = 12$) and $A_{Fe} = 7.54 \pm 0.03$, respectively. These results agree with the meteoritic value $A_{Fe} = 7.51 \pm 0.01$ (Anders & Grevesse 1989), but are in conflict with "high" abundances $A_{Fe} = 7.78 \pm 0.06$ and $A_{Fe} = 7.66 \pm 0.06$ determined from Fe II lines by Babii et al. (1989) and Pauls et al. (1990), respectively. The solar iron abundance obtained from photospheric Fe I lines with the Oxford gf values is substantially higher than the meteoritic one: $A_{Fe} = 7.67 \pm 0.02$ (Blackwell et al. 1984), $A_{Fe} = 7.64 \pm 0.03$ (Gurtovenko & Kostik 1989), and $A_{Fe} = 7.63 \pm 0.04$ (Rutten & van der Zalm 1984, Rutten & Zwaan 1983).

In 1991, the abundance determination from Fe I lines by Holweger et al. appeared to have solved this controversy. Their work is based on new gf values by Bard et al. (1991) which agree rather well with the Oxford values

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(Blackwell et al. 1979, 1982a,b,c, 1984, 1986) with a small difference of 0.034 dex. The "low" $A_{Fe} = 7.50 \pm 0.07$ is only 0.02 dex larger than the one derived earlier by Holweger et al. (1990) from lines of Fe II and is very close to the meteoritic value.

However, why the resulting solar iron abundances of Holweger et al. (1991) and Blackwell et al. (1984) deviate appreciably more (0.17 dex) than their gf scales is a puzzle. Holweger et al. (1991) identified one source of discrepancy: the solar microturbulence ξ. Different values were adopted by Holweger et al. (1991) and Blackwell et al. (1984) (1 and 0.845 km s^{-1}, respectively). But the choice of ξ explains only part (0.05 dex) of the total discrepancy, whose explanation is the main topic of our paper.

Table 1. Input data and results from Kiel and Oxford for the four Fe I lines

λ	E.P.L.	Holweger et al. (1991)			Blackwell et al. (1984)		
		W	log gf	A	W	log gf	A
(nm)	(eV)	(pm)		$\xi = 1.0$	(pm)		$\xi = 0.845$
				E = 2.0			E = 1.2
608.27	2.22	2.82	-3.59	7.48	3.40	-3.57	7.607
675.01	2.42	7.70	-2.61	7.60	7.58	-2.62	7.655
694.52	2.42	8.20	-2.44	7.50	8.38	-2.48	7.658
697.88	2.48	7.90	-2.48	7.54	8.01	-2.50	7.655
$\bar{A}$				7.53			7.644

Table 2. Kiev calculations for the lines of Table 1

λ		gf- Kiel				gf-Oxford	
	W	Kiel	Kiel	Oxf.	Kiel	Kiel	Oxf.
(nm)	E	Kiel	Kiel	Kiel	Oxf.	Kiel	Oxf.
	ξ	Kiel	Oxf.	Kiel	Kiel	Kiel	Oxf.
608.27		7.481	7.492	7.605	7.484	7.461	7.606
675.01		7.595	7.655	7.574	7.640	7.605	7.689
694.52		7.497	7.564	7.537	7.552	7.537	7.697
697.88		7.538	7.599	7.561	7.584	7.558	7.692
$\bar{A}$		7.528	7.578	7.569	7.565	7.540	7.671

2. Discussion

Another discrepancy noted in the literature is the anomalous behavior of those Fe I lines with lower excitation energies near ~2.2 eV obtained by the Oxford group (Blackwell et al. 1984). The iron abundances from these lines appeared to be lower on average by 0.06 dex than for the other lines in their sample.

Table 1 compares the iron abundance results for the four lines in common between the analyses of Holweger et al. (1991) and of Blackwell et al. (1984). The mean abundances from Oxford and Kiel for these four Fe I lines differ by $\Delta A = 7.644 - 7.53 = 0.114$ dex which exceeds the difference in logarithmic oscillator strengths by one order (≈ 0.01).

To explain this discrepancy we test the effects of using different input parameters one at a time. The same LTE line fitting technique for W (equivalent width) and the model HOLMUL are used. The results are listed in Table 2. We decrease ξ to the value used by Blackwell et al. (1984) (Table 2, columns 3 and 2), we adopt the Oxford equivalent widths (Table 2, columns 4 and 2), and we reduce the factor E from 2.0 to 1.2 (Table 2, columns 5 and 2). The sum of all abundance changes, ΔA_i, including the effects of differences in gf and uncertainties due to inconsistencies in the computer codes of Oxford and Kiel amounts to $\Delta A_S = 0.050 + 0.041 + 0.037 + 0.012 - 0.027 = 0.113$ dex. It coincides within rounding errors with ΔA found from Table 1. Thus, for the particular case of our four lines, the large discrepancy between the abundances, despite small differences in gf values, is the sum of the uncertainties in the parameters ξ, W, *E*, and of computer code inconsistencies.

What are the code inconsistencies? Our code (hereafter Kiev) reproduces the Kiel abundances rather well within 0.01 dex (Table 2, column 2 and Table 1, column 4). The Oxford results obtained with the Kiev code differ by up to 0.039 dex (last columns of Tables 1 and 2) which is sufficiently large to justify further study.

Table 3. Iron abundances obtained at Kiev from 19 Fe I lines. The line list, lower E.P., and log gf are taken from Blackwell et al. (1984), $\xi = 0.9$ km s^{-1}, $E = 1.2$

λ (nm)	E.P.L. (eV)	W (pm)	log gf Oxford	A	λ (nm)	E.P.L. (eV)	W (pm)	log gf Oxford	A
444.54	0.09	3.65	-5.44	7.599	635.38	0.91	0.15	-6.48	7.656
519.87	2.22	9.96	-2.13	7.707	649.49	2.39	16.2	-1.27	7.553
540.57	0.99	25.1	-1.84	7.641	649.89	0.96	4.35	-4.70	7.653
543.45	1.01	19.0	-2.12	7.630	662.50	1.01	1.39	-5.37	7.653
606.54	2.61	12.0	- 1.53	7.613	675.01	2.42	7.53	-2.62	7.653
608.27	2.22	3.40	-3.57	7.601	832.70	2.20	18.2	-1.53	7.598
612.02	0.91	0.47	-5.97	7.671	838.77	2.18	20.0	-1.49	7.655
613.66	2.45	13.9	-1.40	7.568	851.40	2.20	12.4	-2.23	7.676
626.51	2.18	8.59	-2.55	7.626	868.86	2.18	27.9	-1.21	7.724
628.06	0.86	5.98	-4.39	7.597				$\bar{A}$	= 7.644

To answer the latter question and to explain the puzzle of Holweger et al. (1991) we investigate the sensitivity of the abundance determinations from the complete Fe I line list to the uncertainties of W, ξ, partition functions, integration of the line profiles, continuous opacity coefficients, and damping constants γ.

3. Results

We divided the abundance determination errors from the Fe I line list of Holweger et al. (1991) into four categories. The errors of the first type are caused by the uncertainties in the partition functions and the profile integration. They are small (0.01 to 0.02 dex). Uncertainties in *E* and hydrogen density yield the second type of error characterized by a steady increase of the errors with W. The abundance errors exceed 0.15 dex for strong Fe I lines. The errors of the third type are due to uncertainties in ξ, observed W, and continuum opacity and reach a maximum ≈ 0.08 dex for the lines of intermediate strengths (W ≈ 8 to 12 pm). The fourth type of error is produced by uncertainties of mean square radii, $\bar{r}^2$, when the Van der Waals damping constant, γ_6, is calculated by classical impact theory. The dependence of the abundance errors on equivalent widths has a forked appearance due to the difference between mean square radii of the dipole approximation of Unsöld (1955) and tabulated ones by Warner (1969) with Thomas-Fermi-Dirac wave functions. The spread of sign-reversed abundance values of the latter type is nearly 0.17 dex whereas the average value is one order smaller. Thus we conclude that the errors in the abundances derived from the equivalent widths of the Fe I lines of Holweger et al. (1991) are due to the uncertainties primarily in *E* and secondly in ξ.

3.1. Puzzle of Holweger et al.

We have derived iron abundance values with the Kiev program for Fe I lines of Holweger et al. (1991) using their gf scale. The microturbulence was taken as the average between that of Holweger et al. (1991) and Blackwell et al. (1984), i.e., 0.9 km s^{-1}. The value of *E* was varied to obtain a range of corresponding abundance values per line. The root mean square errors, ε, in the average abundances $\bar{A}$ have then been calculated per line list and for the set of *E*. Figure 1 (left panel) displays the dependence of ε on the corresponding values *E* and $\bar{A}$. The minimum of this curve shows the preferred combination of *E* and $\bar{A}$ for this line list; $A_{Fe} = 7.50 \pm 0.07$ and $E = 1.9$.

We have similarly redetermined the iron abundance using 19 Fe I lines from other Oxford measurements (Blackwell et al. 1979, 1982a,b,c, 1984, 1986), their gf values and $\xi = 0.9$ km s^{-1} (Table 3 and Figure 1, right panel). The values of W in Table 3 are taken from Gurtovenko & Kostik (1989). The line selection is comparable in its W and wavelength ranges to the Kiel line list. Unfortunately, the similarity breaks down for the excitation energy because of the lack of high-excitation lines in the Oxford data. The minimum value of ε for the Oxford list is at a mean abundance, $A_{Fe} = 7.64 \pm 0.04$ and $E = 1.2$.

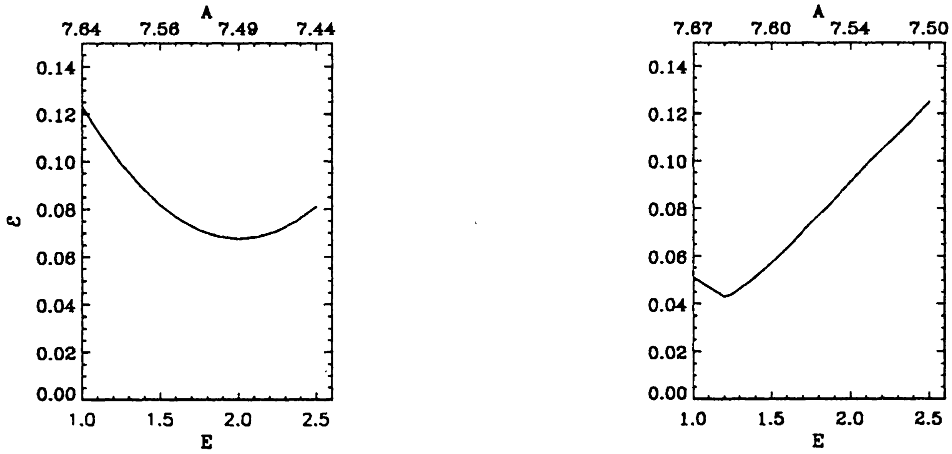

Fig. 1. Dependence of root mean square error variation, ε, on the damping enhancement factor, E. The corresponding values of $\bar{A}$ are indicated along the top. Left: Fe I lines and gf values from Holweger et al. (1991). Right: Fe I lines and gf values from Blackwell et al. (1979, 1982a,b,c, 1984, 1986). The minima define the "best" choice of E

Thus, the most probable values of abundances derived from the gf scales of Kiel and Oxford are obtained with quite different E values, i.e., 1.9 and 1.2, respectively. This difference explains most of the Kiel-Oxford abundance discrepancy. Comparing the two panels in Figure 1 at a given E demonstrates that the discrepancy is small. Taking into account the difference of 0.034 dex in gf scales such comparison shows that $\Delta A = 0$ and 0.03 for $E = 1$ and 2.5, respectively. The slight increase of the abundance discrepancy with E may be due to the difference in excitation potential sampling between the two line lists.

3.2 Abundance Anomaly for 2.2 eV Fe I Lines

The discussion of errors in the abundance determinations shows that the lines of Fe I with excitation potentials of lower level *E.P.* $\sim$ 2.2 eV are sensitive to the evaluation of the mean square radii, $\bar{r}^2$. We have determined the iron abundance with the Kiev code using the 25 Oxford Fe I lines of Blackwell et al. (1984) and their input data for two cases. In the first one $\bar{r}^2$ were evaluated according to dipole approximation of Unsöld (1955). In the second case the mean square radii tabulated by Warner (1969) from Thomas-Fermi-Dirac wave functions have been used. Close agreement of the abundance values derived for the first case with the results of Blackwell et al. (1984) (differences ≤ 0.008 dex) shows that the Oxford group quite likely employs the Unsöld dipole approximation for $\bar{r}^2$ rather than other methods such as Warner (1969). This practice explains most of the code-to-code differences of Kiev and Oxford. Figure 2 more clearly illustrates the effect of $\bar{r}^2$. A sizable dip obtained by Blackwell et al. (1984) for lines with lower-level excitation potentials near

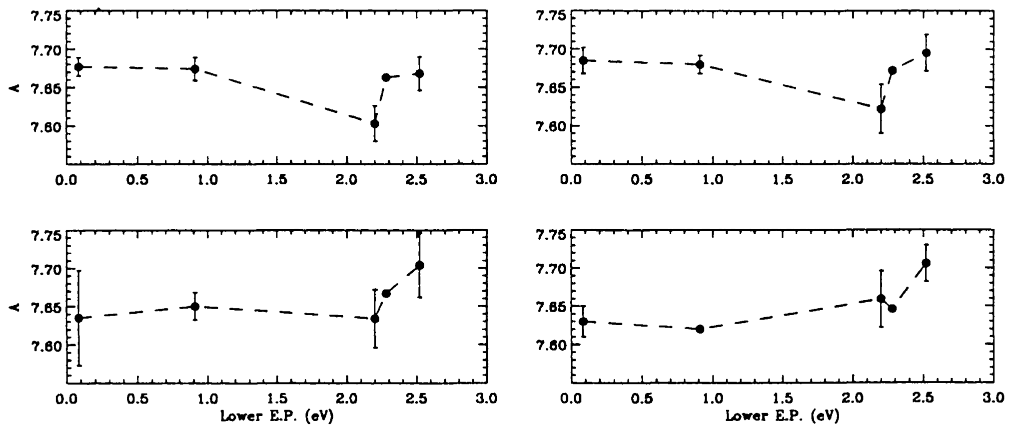

Fig. 2. Iron abundances averaged over lines of similar lower-level excitation potential (E.P.) for the 25 lines from Blackwell et al. (1984). Error bars are rms variation. Upper left panel: results of Blackwell et al. (1984). Upper right panel: fits for equivalent widths of Blackwell et al. (1984). Lower left panel: fits for equivalent widths of Gurtovenko & Kostik (1984). Lower right panel: fits for equivalent widths of Rutten & van der Zalm (1984). The collisional damping for the fits is computed with the mean square radii of Warner (1969).

E.P. = 2.2 eV shown in the upper left panel slightly decreases when mean square radii of Warner (1969) are used.

We now consider the observed equivalent widths since this can be a sensitive parameter. The equivalent widths of Gurtovenko and Kostik (1989) make the dip near 2.2 eV less significant (Figure 2, lower left panel). Its depth is smaller now than the root mean square variations of abundance. The dip actually is absent in the lower right panel when equivalent widths of Rutten & van der Zalm (1984) are employed. Thus, these results support the conclusion about the statistical insignificance of the anomaly for 2.2 eV Fe I lines.

4. Conclusions

The significant discrepancy of abundances obtained with the similar gf scales of Kiel and Oxford is connected with the use of different values for *E*. However, the removal of the contradiction does not allow to answer definitively the questions: Which scale of gf is preferable? What is the value of *E*? Finally, what value of solar iron abundance is correct, viz. a "low" or "high" one? Indirect evidence in favour of the "high" results based on the Oxford scale of gf are the smaller root mean square error in abundance ($\varepsilon = \pm 0.04$ dex whereas for the Kiel scale $\varepsilon = \pm 0.07$ dex) and a more pronounced minimum of the function $\varepsilon(E)$ in comparison with Kiel results. To clarify the above dilemma, further investigations are needed which allow for the inhomogeneities of the solar atmosphere and NLTE effects. More reliable theoretical damping enhancement factors are required as well, due to the high sensitivity of the empirical values to the uncertainties of gf scales.

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