# LIMITATIONS OF STELLAR ABUNDANCE DETERMINATIONS

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ABSTRACT. The information content of (photospheric) stellar spectra and the accuracy of abundance determinations are discussed. Besides the physical properties of the line spectra, the spectral resolution, the signal-to-noise ratio, but also the incompleteness of the knowledge of the contributing blends limit the abundance information. For a perfect model atmosphere the main factors determining the accuracy of the abundances are S/N, the line saturation, and the location of the continuum (or, in a synthetic spectrum, the background of numerous lines). In addition systematic errors introduced by missing atomic data and an imperfect model atmosphere (non-LTE, line blanketing, hydrodynamics) are important. The typical accuracy of abundance determinations is discussed for main sequence stars for which the most reliable data are available, and for a few selected other stellar types.

## 1. Motive

The *atmosphere* (photosphere, shell ...) is by definition the directly observable part of the star, producing its *spectrum*. Usually the mass of the atmosphere is a tiny fraction of the stellar mass, and hence the atmosphere is 'vulnerable' to changes during the star's evolution. In particular changes of the element composition $\varepsilon_\alpha$ may arise. We write the atmospheric abundance $\varepsilon_\alpha(t)$ for each element $\alpha$ at a time t as the sum of the composition at birth $\varepsilon_\alpha(0)$ plus the abundance change $\delta\varepsilon_\alpha(t)$. The following basic types of $\delta\varepsilon_\alpha(t)$ may be distinguished:

*'Internal'* origin, i.e. arising within the star itself:

(a) *nuclear* ⇒ products of nuclear reactions appearing at the surface due to convection, meridional circulation, stellar wind, ejection of matter (novas, supernovas), ...

(b) *non-nuclear* ⇒ separation of elements, e.g. by diffusion, radiation pressure, ...

*'External'* origin:

accretion of matter by a close companion or from the interstellar medium, spallation by cosmic rays, ...

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Since $\delta\varepsilon_\alpha(t)$ as well as $\varepsilon_\alpha(0)$ have to be inferred from theory, the analysis of stellar spectra yields valuable information for our understanding of stellar evolution and formation, and a discussion of the amount of information and the accuracy which can be achieved is of prime interest.

In this contribution the discussion will be restricted to the analysis of the *photospheric* spectra of *single* stars.

## 2. Information Content of a Stellar Spectrum

Naturally, the ideal case would be to determine the abundances of all the roughly 285 'stable' nuclides with a half-life $\geq 10^{10}$ yr. The information about *isotopes*, however, is very limited even in sharp-lined spectra. For atoms and ions the wavelength differences for the isotopes are determined by the differences in the reduced masses of nucleus $m_A$ and electron $m_e$ which are small since $m_e \ll m_A$ . Essentially only abundances of $^1$H $^2$D, $^{3,4}$He, and $^{6,7}$Li can be obtained. For molecular spectra the situation is more favourable, but the formation of molecules is restricted to relatively cool or dense plasmas. In addition, in a few cases the nuclear spin yields information on isotopes via the hyperfine structure. Thus in general we can derive abundances for at most some 90 elements (nuclides).

The *observational parameters* of a spectrum are (a) the spectral resolution $\lambda/\Delta\lambda$ and (b) the signal-to-noise ratio S/N. The spectral resolution has only to be sufficient to resolve the narrowest structures given by rotation, turbulence or differential expansion. On the other hand, S/N should be as large as possible for gaining maximum information.

Additional observational parameters such as time resolution (for variable stars) and spatial resolution (granulation, star spots) are not considered here.

In principle, if $S/N \to \infty$, an abundance determination is possible for any extremely rare trace element from very faint features or 'bumps' in the synthetic spectrum provided the properties of the atmosphere such as the stratifications of temperature, electron density etc. are known.

For the Sun, the best analyzed star, the lowest abundances derived are of the order of $\varepsilon_\alpha \simeq 10^{-12}$, e.g. for Ho, Tm, Tb, Ta. Here and in the following abundances are defined as number densities relative to hydrogen, $\varepsilon_\alpha = N(\text{element } \alpha)/N(H)$. On the other hand, for near main-sequence B stars in the Magellanic Clouds $\varepsilon_\alpha \geq 10^{-5}$ for Al is reached.

*In practice* the abundance determination is limited by the wavelength positions of the most favourable lines and by the degree of crowding of lines. If a line is not located in a spectral range where the photospheric flux is strong, the accuracy of the derived abundance is not too high. Furthermore, the evaluation of a faint 'bump' by the spectrum synthesis techniques requires knowledge of *all* neighbouring absorption line blends.

A crude estimate suffices to illustrate the role of the background due to numerous weak lines. Kurucz' (1990) list contains some $10^7$ lines with e.g. $6.1 \cdot 10^6$ lines of singly ionized iron-group elements (Ca-Ni) of which $1.2 \cdot 10^6$ are due to Fe II. If we assume that $2 \cdot 10^6$ lines fall in the wavelength range from 0 to 20000 Å, the line density is 100 lines/Å. On the other hand, lines of a Doppler velocity of 3 km $s^{-1}$, corresponding to a width w = 0.05 Å at 5000 Å, are densely packed already for a density of 20 lines/Å. The majority of lines therefore forms a 'wavy' ***quasi-continuum*** with fluctuations given by the square root of the line density having little resemblance to the wavelengths and strengths of the many individual lines. This background problem increases with increasing line width (e.g. for rotating stars or supernovas). As an example for the contribution to the line density by lines of different strengths, the distribution of Fe II lines in their resonance region (2000-2600 Å) is shown by Baschek (1990).

There are, however, also fairly line-free ranges, such as the optical region of early-type stars, which allow more accurate abundance determinations.

Incidentally, also the 'real' continua or photo-ionisation cross sections can exhibit considerable structures, e.g. those of O I (cf. Butler, 1990) or Fe I (Hansen et al., 1977).

## 3. Accuracy of Abundances — Ideal Model Atmosphere

We first assume that the atmospheric stratifications of temperature, pressure, absorption coefficients etc. are perfectly known.

The ***observational*** limitations have been analyzed by Landman et al. (1982) and Cayrel (1988). For a Gaussian line profile with Doppler width $\Delta\lambda_D = \sqrt{2}$ w the accuracy of the equivalent width $W_\lambda$ is given by

$$\sqrt{\langle \Delta W_\lambda^2 \rangle} = \sqrt[4]{(9\pi)} \cdot \sqrt{w \delta x} \cdot \eta,$$

where $\delta x$ is the pixel size and $\eta$ the r.m.s. relative photometric accuracy of the flux (c: continuum)

$$\eta = \sqrt{\langle \Delta F^2 \rangle} / F_c \simeq (S/N)^{-1}.$$

This yields, e.g., for $\delta x$ = 35 mÅ, w = 40 mÅ, and S/N = 100 an error of $\langle \Delta W_\lambda^2 \rangle^{1/2}$ = 0.8 mÅ. This result is too optimistic since the location of the continuum is assumed to be known and no blends are considered.

A more realistic error estimate for the equivalent width is

$$\sqrt{\langle \Delta W_\lambda^2 \rangle} = 6 \text{ w} \cdot \eta,$$

*in*dependently of $W_\lambda$. For $\eta = 0.005$ and w = 40 mÅ, $\Delta W_\lambda \simeq 1.5$ mÅ. Here the relative accuracy $\Delta W_\lambda/W_\lambda$ decreases with $W_\lambda$; e.g. $\Delta W_\lambda/W_\lambda \simeq 0.10$ for $W_\lambda = 15$ mÅ. Hence for faint lines

$$\frac{\Delta\varepsilon}{\varepsilon} = \frac{\Delta W_\lambda}{W_\lambda}$$

holds.

On the other hand, ***theoretical*** limitations prevent an increase of the accuracy with increasing equivalent width above about 10 per cent. If the optical depth $\tau$ in the line center becomes of the order of 1, i.e. if ***saturation*** on the flat part of the curve of growth is reached, $W_\lambda$ is less sensitive to the abundance, and in addition depends on the microturbulent velocity. According to Cayrel (1988) an ***optimum accuracy*** is achieved from lines with $W_\lambda \simeq 20$ mÅ, yielding $\Delta\varepsilon/\varepsilon \simeq 0.1$ or $\Delta \log\varepsilon \simeq 0.04$ dex.

For a line e.g. at 3000 Å with a Doppler velocity of 3 km $s^{-1}$, the condition for saturation, $\tau = 1$, neglecting atmospheric structure effects corresponds to $\varepsilon \text{ f } \zeta \simeq 3 \cdot 10^{-12}$ where $\zeta = N_i / \sum N_i$ is the degree of excitation/ionisation (Baschek, 1984).

Since $W_\lambda$ depends on the product of abundance $\varepsilon_\alpha$ times *oscillator strength f*, the errors in the abundances depend also on the uncertainties of the f values. The accuracy of atomic transition probabilities on the basis of the comprehensive material available at the National Institute of Standards and Technology (NIST), formerly National Bureau of Standards (NBS), is discussed by Wiese and Fuhr (1990). The following simplified Table summarizes the typical accuracy of atomic f values for six groups of spectral lines.

| [dex ] | stronger lines<br>f > 0.01 | weaker lines<br>f < 0.01 |
|---|---|---|
| simple atoms<br>*(1 or 2 electrons)* | < 0.04 | 0.10 |
| moderately complex atoms<br>*( e.g. C, N, O, Al )* | 0.04 ... 0.06 | 0.18 |
| complex atoms | < 0.10 | 0.18 ... >0.30 |

For example, a comparison between experimental data from the NIST (NBS) compilation with Kurucz' (1981) semi-empirical calculation for Fe II shows agreement generally within ±0.18 dex (±50% ) for the stronger lines with log gf > −0.18 (Wiese and Fuhr, 1990).

Oscillator strengths are *not* needed in a strictly *differential* analysis, i.e. if — for a given model atmosphere — the abundances of a star are determined relative to those of a comparison star of similar type. Very strong lines depend also on the damping constants entering the line profile.

## 4. Accuracy of Abundances — Realistic Model Atmosphere

Besides the random errors inherent in the observed spectra ($\Delta\lambda/\lambda$, S/N) and in the atomic data (f values, ...) the accuracy of the abundances is also strongly affected by *systematic* errors which are very difficult to assess. Here essentially *missing atomic data* and *imperfect model atmospheres* contribute although the basic physics is known and large computers are available. A discussion of these aspects is given e.g. in the review by Mihalas (1990). It may suffice here to mention only some problems:

*Non-LTE calculations*: A large amount of atomic data (f values, cross-sections, ...) is needed, much larger than for calculations in LTE. It is vital to any non-LTE treatment that all relevant reaction channels are included.

*Line Blanketing*: The calculation of static model atmospheres in LTE already requires inclusion of some $10^6$ or more lines by statistical or sampling methods. Considerable difficulties arise if blanketing by lines is to be treated in non-LTE although suitable numerical schemes have been developed. Also (differentially) moving atmospheres pose problems with the line blanketing.

*Hydrodynamics*: The exact treatment of the manifold of phenomena connected with 'hydrodynamic' processes (in a wider sense), coupled to a radiation field, is beyond the present day possibilities. Sufficiently fast 2D and 3D hydrodynamical codes are not available in general. Thus the occurrence of microturbulence, granulation, convection, stellar winds etc. introduces uncertainties in the model atmosphere and hence in the element abundances.

As a consequence of these uncertainties the best abundance data that can be obtained are those for stars on or near the main sequence of types B to G. Here the atmospheres are compact, the non-LTE effects are not too pronounced, no winds occur, and hydrodynamic processes are not dominating. Hence the errors in the model parameters and the abundances are smallest.

A general determination of the uncertainties of the element abundances, i.e. a systematic *sensitivity analysis*, is not yet available. A promising formalism to deal with the general problem has been suggested by Wehrse (1990): Assuming that all atmospheric parameters are closely connected, a 'super-vector' $\mathbf{X} = \{\mathbf{p}, \varepsilon, \mathbf{q}\}$ is constructed in which $\mathbf{p}$ comprises the atmospheric parameters effective temperature, surface gravity, and microturbulent velocity, $\varepsilon$ contains the abundances of e.g. 92 elements, and $\mathbf{q}$ the relevant input physics, in particular the f values. The corresponding error vector is $\Delta\mathbf{X} = \{\Delta\mathbf{p}, \Delta\varepsilon, \Delta\mathbf{q}\}$. The emergent flux $F_\lambda$, i.e. the *spectrum*, can now formally be expressed by

$$F_\lambda = F_\lambda(\mathbf{X}),$$

and its errors by

$$\Delta F_\lambda = \frac{dF_\lambda}{d\mathbf{X}} \Delta\mathbf{X}.$$

These relations are determined by the equations for hydrostatic and radiative/convective equilibrium, radiative transfer, the equation of state, the absorption coefficients etc. The $\Delta F_\lambda$, determined from the S/N ratio are regarded as given at a set of wavelength points. Finally, we obtain for the abundance errors

$$\Delta\varepsilon = \left(\frac{dF_\lambda}{d\varepsilon}\right)^{-1} \cdot \left(\Delta F_\lambda + \frac{dF_\lambda}{d\mathbf{p}}\Delta\mathbf{p} + \frac{dF_\lambda}{d\mathbf{q}}\Delta\mathbf{q}\right).$$

All matrices in this expression can be evaluated analytically so that the sensitivity analysis can be carried out, the expressions are, however, complicated (Wehrse, 1990).

## 5. Accuracy of Abundances — Examples for Various Stellar Types

The accuracy of abundance determinations for stars near the *main sequence* has been reviewed recently at the General Assembly of the IAU in Baltimore 1988 by Mendez (1990) for O to mid-B stars, by Sadakane (1990) for middle B to F stars, by Spite (1990) for solar-type stars, and by Bessell and Scholz (1990) for K and M dwarfs.

In the B stars helium can be determined within 0.08 dex, while elements such as C, N, O, Mg, Al, Si have an accuracy of about 0.3 dex. In O stars, He can be determined fairly accurately (about 0.1 dex), but the other elements are uncertain by at least a factor of 3. The accuracy is mostly limited by the treatment of non-LTE, blanketing, and stellar winds.

For the A and F stars the abundance of Fe, an abundant element with many lines, in general is accurate within about 0.3 dex, for the G stars somewhat better (about 0.2 dex). The results for the well studied star Vega have an error of ±0.2, and for the Sun of ±0.1 dex. Besides the uncertainties in the non-LTE calculations, uncertainties in atomic data, in the effective temperature, and in the microturbulent velocity determine the abundance errors.

In the late-type dwarfs very accurate abundance determinations are not yet possible. Convection, molecule formation and molecule opacities cause uncertainties in the abundances by a factor of 3 or more.

The accuracy of a *differential* analysis, star compared to comparison star, is higher. An even better accuracy can be obtained if abundance *ratios* of elements of similar ionisation and excitation characteristics are derived, e.g. (Ni/Fe) *vs.* (Ni/Fe) in the comparison star.

Finally, some comments on a few selected stellar types are given.

(1) The *Wolf-Rayet stars* are an important group displaying abundance changes due to stellar evolution (mixing, mass loss) and nucleosynthesis.The analysis of their optically thick, extended and moving atmospheres poses problems resulting in not

too accurate abundances (He, C, N, O) of about $\simeq \pm 0.5$ dex (e.g. Nugis 1982, Willis 1982 a,b, Hillier 1987).

(2) Among the *A-type stars* the standard *Vega* has been analyzed independently by several authors. Their abundance determinations for Fe agree to within 0.15 dex, a major source of error are the non-LTE effects in the ionisation equilibrium Fe I/Fe II (cf. Sadakane, 1990).

As an example for an interesting group of peculiar stars we mention the ***Lambda Bootis stars.*** Recent analyses of these metal-deficient stars point out similarities to the Vega-type stars (Baschek and Slettebak, 1988, Venn and Lambert, 1990). Is $\lambda$ Boo a rotating Vega, or Vega a mild $\lambda$ Boo star? Since for the $\lambda$ Boo stars v $\sin i \simeq 100$ km $\mathrm{s}^{-1}$, their abundances are less acurate than those of the sharp-lined A stars. The different metal abundances in $\lambda$ Boo and Vega lead to different ultraviolet fluxes and hence possibly to systematically different non-LTE effects. When discussing the abundance pattern of $\lambda$ Boo one further should keep in mind that the by far strongest feature in its spectrum, the broad absorption at $\lambda 1600$ Å, is not yet understood (Baschek et al., 1984, Jaschek et al., 1985).

(3) For *M dwarfs* the overall energy distribution can be reproduced by model atmospheres reasonably well, but no accurate abundances can yet be determined, the errors being at least $\pm 0.5$ dex. Details of the state of the art can e.g. be found in the recent analysis of Gliese 866 ($T_{\mathrm{eff}} = 2900$ K) by Leinert et al. (1990).

(4) The accuracy of abundance determinations from high-resolution *extragalactic spectroscopy* may be illustrated by the analyses of essentially unevolved B stars with V $\simeq 14$ mag in blue globular clusters of the Magellanic Clouds (Reitermann et al., 1990, Jüttner et al., 1989, 1990). From blue CCD spectra with a resolution of $2 \cdot 10^4$ and S/N $\leq 100$, taken with CASPEC at the 3.6 m telescope of ESO, abundances of He, C, N, O, Mg, Al, Si, S, and Fe can be obtained with an accuracy of $\pm 0.2$ to $\pm 0.3$ dex, where the uncertainty is largely due to the ill determined microturbulence.

## 6. Summary and Outlook

The information contents of stellar spectra and the accuracy of element abundances $\varepsilon_\alpha$ have been discussed with emphasis on the problems typical for high-resolution observations.

The most accurate abundances can be determined for stars on or near the main-sequence. In the most favourable cases, for the Sun and for Vega, and for the helium abundance of early-type stars, an accuracy of $\simeq \pm 0.1$ dex can be achieved. With the exception of O and M stars the errors for main-sequence stars are typically $\pm 0.2$ to $\pm 0.3$.

For many stellar types relevant to stellar evolution problems, abundances can be obtained with medium accuracy ($\pm 0.2 \ldots \pm 0.3$), but for some interesting groups such as Wolf-Rayet stars, novas, and supernovas, only about ±0.5 or even less can be reached.

On the one hand it is important to study bright stars with S/N $\rightarrow \infty$ with the highest perfection of models in order to remove systematic errors. On the other hand, there are many 'interesting' stars for which abundance investigations are valuable even if the accuracy of their $\varepsilon_\alpha$ is not too large, e.g. due to model atmosphere problems for evolved stars or to low $\lambda/\Delta\lambda$ or S/N for faint and distant stars.

Even abundance data with an accuracy of ±0.3 can contain much information which is yet to be interpreted in the context of stellar evolution.

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