On the Abundances of Li, Be and O in Metal-Poor Stars in the Galaxy

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Abstract
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Stellar atmospheres constitute excellent environments to study the chemical evolution of our Galaxy. The chemical composition of these atmospheres reflects the composition of the gas from where these stars were born. As the Galaxy evolves, the composition of the gas changes from being primordial (Big-Bang nucleosynthesis) to being enriched in heavy elements (stellar and interstellar nucleosynthesis). The abundances of fragile chemical elements can be affected by stellar mixing processes. Precise lithium, beryllium and oxygen abundance determinations in old stars are presented in this thesis. These determinations are based on the analysis of the observed spectra of a sample of thirteen metal-poor subgiant stars. According to stellar mixing theories, these stars are in a stellar evolutionary stage in which mixing by convection is expected. Abundances of fragile elements like lithium and beryllium are thus expected to be affected by such mixing processes. As a consequence of this, the abundances of these elements are discussed in a dilution context. Lithium and beryllium abundances are compared with the abundances of stars with similar characteristics but in a less evolved stellar phase so that mixing processes have not acted yet. As expected, our abundances seem to be depleted following reasonably well the standard predictions. Stellar abundances of oxygen should give an estimate of the oxygen contribution of core-collapse supernovae to the interstellar medium. However, there is poor agreement among the abundances determined from different atomic or molecular indicators in general. Abundances coming from three different indicators are compared in this thesis. The abundances determined from the O i infrared triplet lines at 777.1-5 nm give the poorest agreement among the three indicators. The abundances based on OH ultraviolet lines around 310 nm are lower for the subgiants in comparison with previous studies of main-sequence stars, becoming even lower than values based on the O i forbidden line at 630.03 nm. Still the most reliable indicator appears to be the O i forbidden line which suggests a plateau-like or only slowly increasing [O/Fe] towards lower [Fe/H]. In addition, the line formation of the Be ii ultraviolet resonance lines at 313.0±1 nm, commonly used for abundance determinations purposes, is investigated under non-local thermodynamic equilibrium. We find that the common assumption of local thermodynamic equilibrium typically gives systematic errors of about 0.1 dex.

Keywords: galactic evolution, stellar abundances, stellar atmospheres, spectral line formation, stellar mixing

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urn:nbn:se:uu:diva-4814 (http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-4814)
A esas otras dos partes de mi ser,
a mi madre y a mi hermano
List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals:

I  A. E. García Pérez, M. Asplund, F. Primas, P. E. Nissen and B. Gustafsson,
“Oxygen abundances in metal-poor subgiants as determined from [O I], O I and OH lines”,
_Astronomy & Astrophysics_ (submitted).

II A. E. García Pérez and F. Primas,
“Li and Be depletion in subgiants”,
_Astronomy & Astrophysics_ (submitted).

III A. E. García Pérez and D. Kiselman,
“Departures from LTE in the formation of the Be II UV resonance lines in late type stars”,
_Astronomy & Astrophysics_ (submitted).

Papers not included in the thesis:

I  M. Asplund and A. E. García Pérez,
“On OH line formation and oxygen abundances in metal-poor stars”,

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1 Introduction

Someone recently told me that the type of introduction of a thesis depends on the age of the author; the older you get the more you dwell on philosophical aspects. This may be right but I guess that it also depends on the person. If you grew up as I did in a place with a wonderful sky, would you not ask yourself about these shining objects before starting to wonder about philosophical matters? Later on, you start to study physics and you realise that you can learn much about these shining objects by applying physical laws, sometimes very simple ones. I was fascinated by the fact that stellar light is not only the source of life but also of knowledge, it can teach us about the nature of these distant objects. And because this was the driving force that put me where I am at the time of writing this thesis, I want to stress and reflect on this capacity of light in this introduction.

The property of light that it separates into different colours (a spectrum) when passing through a prism was discovered by Isaac Newton (1643-1727). Later, Joseph Fraunhofer (1787-1826) and others observed dark lines in the spectrum of the Sun for the first time. John Herschel (1792-1871), in a groundbreaking discovery, realised that by analysing flame spectra, the composition of these flames was reflected in their spectra.

"While we can conceive of the possibility of determining their shapes, their sizes, and their motions, we shall never be able by any means to study their chemical composition or their mineralogical structure ... — Auguste Comte, Cours de la Philosophie Positive, 1835."

My working place during the last years is named after the Uppsala physicist Anders Jonas Ångström (1814-1874) who made a beautiful atlas of the solar spectrum and proved the existence of hydrogen in Sun, while Gustav Robert Kirchhoff (1824-1887) was one of the first to establish the presence of solar magnesium (Mg), calcium (Ca) and iron (Fe) among other elements studying the solar spectra. These studies were extended to other stars by Angelo Secchi (1818-1878) and William Huggins (1824-1910).

Already in the beginning of the last century, several scientists started studying the formation of spectral lines. It was Marcel G. J. Minnaert (1893-1970)
who introduced terms like equivalent width from which abundances\(^1\) can be estimated; this concept will be introduced below.

Stellar abundance studies date since then. For the chemical elements under discussion in this thesis, oxygen\(^2\) (O), lithium (Li) and beryllium (Be), studies in metal-poor stars had their beginnings in the second half of the last century. These stars are old stars with very low contents of elements heavier than hydrogen and helium, of so-called metals.

The construction of 8 m telescopes and highly efficient spectrometers has significantly reduced observational errors in the abundance determinations and pushed down the detection limit of weak spectral lines. In this thesis, we have made use of the capabilities of the Very Large Telescope (VLT) at the European Southern Observatory (ESO) with the aim of determining accurate lithium, beryllium and oxygen abundances for stars of low metallicity. These abundances may help us to better understand the early Galactic chemical evolution of these elements. They also set some constraints on the matter density in the early Universe, on the globular cluster ages as well as on Galactic chemical evolution in general which also entails properties of supernova explosions.

The project is a continuation of a project initiated by Martin Asplund, Poul Erik Nissen and Francesca Primas. Martin Asplund suggested to extend their abundance studies to subgiant stars. Paper III arose because of the need of the group to have accurate determinations of Be abundances. My contribution to the papers is the following; I took part in the observations and analysis of the spectra of Paper I and Paper II and of the NLTE calculations in Paper III. The writing of the three papers in the thesis was almost entirely my task. The discussions in these papers, in particular on 3D effects on stellar abundance determinations, has benefited greatly through contribution from my coauthors. NLTE abundance corrections for the O I triplet lines and the atomic model for beryllium were provided by them. The chapter entitled “In Swedish”, originally written by me in English, was translated into Swedish by Martin Asplund and Emma Olsson.

\(^1\)\(\log \varepsilon(X) = \log N(X)/N(H)\), \(N(X)\) is the number of atoms of the element \(X\).

\(^2\)Oxygen was discovered independently in 1772-73 by the Uppsala chemist Carl Wilhelm Scheele and in 1774 by Joseph Priestley. A few thousand kilometers south and a few years later the French chemist Nicolas-Louis Vauquelin discovered Be in 1798, which was isolated later by Friedrich Wöhler and Antoine Bussy in 1828. The discovery of Li has also its origins in Sweden, more precisely on Utö in the Stockholm archipelago, by Johan August Arfvedson in 1817.
2 Origin and evolution of Li, Be and O

2.1 Production

What is the origin of the matter we are made of? The answer to this question has been pending during the history of the modern astronomy. In the 1940’s and thanks to the pioneering work of George Gamow and collaborators, the elements in the Universe were conceived to originate in Big-Bang nucleosynthesis which took place a few minutes after the explosion. However, the theory only worked for the production of the lightest elements because elements with atomic weights between 5 and 8 are unstable. Hydrogen (H) followed by helium (He) are the most abundant elements in the Universe (about 75% and 25% in mass, respectively). He and the deuterium isotope of H seem to have been produced during the early phases of the Universe, just after the Big-Bang explosion. In smaller amount, $^7\text{Li}$ was also produced. Stellar nucleosynthesis was proposed by Fred Hoyle in the 1940’s and was well established at the end of the 1950’s thanks to the two very important papers by Burbidge et al. (1957) and Cameron (1957). Elements such as oxygen are believed to have been formed in the interior of massive stars ($>10\, \text{M}_\odot$) as a result of nuclear reactions, $\alpha$-particles ($^4\text{He}$) reacting with carbon nuclei. When later on these stars exploded as core-collapse supernovae (supernovae Type II) they enriched the interstellar medium (ISM) with these newly synthesised elements and this enrichment is reflected in the chemical composition of subsequent generations of stars. Models of galactic chemical evolution have been made (see, e.g., Schmidt (1963); Truran and Cameron (1971); Audouze and Tinsley (1974); Tinsley and Larson (1978)). Such models require knowledge about how many stars of different masses are formed per time unit; in astrophysical terms the initial mass distribution (IMF) and the star formation rate (SFR) have to be known or assumed. The contributions (so-called yields) of heavy elements from these massive stars to the ISM depend on supernovae properties such as the mass they retain after the explosion (i.e. their mass cut), the mass loss because of winds etc. and the rates of the nuclear reactions. As the Milky Way Galaxy evolved an increasing number of core-collapse supernovae enriched the ISM and thus increased the oxygen abundance. At the same time, iron abundances also increased as a result of the supernova contribution. When the age of the Galaxy was such that the iron contribution from more slowly evolving thermonuclear supernovae (supernovae Type Ia) took over, the observed
oxygen and iron had different sources of production and varied differently. The ratio of stellar oxygen versus iron abundances measured as relative to the Sun ([O/Fe]) is expected to stay more or less constant until the thermonuclear supernovae started to dominate the iron production. This occurred when the metallicity, often measured as [Fe/H]$^1$ reached a value of about $-1.0$. For higher values of metallicity than this, a decrease for [O/Fe] with increasing [Fe/H] is expected.

For a long time it remained an open question how light elements such as Be and B were produced. Due to their fragile nature, these elements are expected sooner to be destroyed in stars rather than to be produced. This does not suggest a stellar production scenario for the light elements. The possibility of spallation in the interstellar medium arose with the measurements of the chemical composition of cosmic rays by Bernard Peters in the 1960’s. The first estimates of production rates based on protons and $\alpha$-particles accelerated by supernova and colliding with carbon and oxygen nuclei in the ISM were presented by Meneguzzi et al. (1971). The few observed stellar abundances of $^7$Li, $^9$Be and $^{10}$B agreed very well with the predictions. According to standard cosmic ray spallation scenarios, oxygen and beryllium are expected to be correlated quadratically ($N(\text{Be}) \propto N(\text{O})^2$) and therefore this is called a secondary production. In the 1990’s observations of Be and B at low metallicity suggested a linear trend rather than a quadratic one which questioned current ideas about the light element production in the early Galaxy. In better accordance with observations at these metallicities, a primary ($N(\text{Be}) \propto N(\text{O})$) mechanism based on the spallation when accelerated carbon and oxygen nuclei collide with protons and $\alpha$-particles has been suggested (see Duncan et al. (1992); Cassè et al. (1995); Parizot and Drury (1999) and references therein). The acceleration of the particles may be produced either by individual or several supernovae in superbubbles.

2.2 Destruction

In the CNO cycle, carbon and oxygen are transformed into nitrogen. Therefore we expect to observe some signs of that cycle at least for intermediate mass stars when this material shows up on the stellar surface. This is expected to happen when the convection zone at the stellar surface reaches internal layers where these elements have been processed and drags them up to the surface. In post red-giant-branch stars in late stages (AGB), mixing by thermal pulses and subsequent convection (third dredge-up) also happens.

Light elements on the other hand, as it was already mentioned, are very fragile and thus prone to be destroyed by thermonuclear reactions and will

$^1[\text{Fe}/\text{H}] = \log \varepsilon(\text{Fe}) - \log \varepsilon(\text{Fe})_\odot$, the $\odot$ symbol stands for the Sun.
show signs of depletion at earlier stellar evolution phases. Li is the most fragile of the three light elements Li, Be and B. Its nuclear-burning temperature is of the order of $2.5 \times 10^6$ K while the higher burning temperatures for Be and B, $3.0 \times 10^6$ K and $5.0 \times 10^6$ K, respectively, make them more stable than Li. As a result of this, the typical composition of a stellar envelope for a star which has not undergone mixing processes is such that Li and Be are distributed in layers. The Li layer is in the outermost thin region of the star while the Be layer is thicker and deeper. Depletion of these elements is expected for stars undergoing mixing processes involving their atmospheres.

It should be mentioned that Li is also produced in late evolutionary stages, e.g. by the Beryllium-transport mechanism in AGB stars (Cameron and Fowler (1971)).
3 Stellar abundance determinations

All the three papers at the present thesis deal with abundance determinations for light elements. Paper I and Paper II address different problems, mainly from an observational point of view, and use the same set of observational data. Paper III has a more theoretical character, as it deals with a problem in spectral line formation.

3.1 Observations

Observations of the weak O I forbidden line at 630.03 nm ([O I]) in the spectra of metal-poor main-sequence stars was an important achievement by 8m telescopes and their high quality spectrographs. Continuing with the work undertaken by Nissen et al. (2002), we observed a sample of 13 metal-poor subgiants with the UVES spectrograph mounted on the Nasmyth B platform of the Kueyen unit of the ESO Very Large Telescope. The stars were selected according to their published metal contents, temperatures and stellar gravities (evolutionary stage) such that low metallicities were preferred and they had effective temperatures ($T_{\text{eff}}$) high enough to make it possible to detect the O I triplet lines at 777.1-5 nm (O I IR) but still surface gravities ($\log g$) low enough as to admit detection of [O I] lines. According to stellar evolution theory, as stars evolve out of the main-sequence they expand and get cooler so that both $T_{\text{eff}}$ and $\log g$ decrease. We covered the whole visible wavelength range from the near ultraviolet (UV) to the near infrared (IR) in order to observe also the OHA 2$\delta$-X 2$\pi$ electronic bands around 310.0 nm and the Be II resonance doublet lines at 313.0-1 nm. The Li I feature at 670.8 nm was covered, as well. The signal-to-noise ratio (S/N) of our co-added spectra was sufficiently high (100 and 500 for the central wavelengths of spectral orders in the blue and red, respectively) that we succeeded in detecting the [O I] and O I IR lines at metallicities as low as $\text{[Fe/H]} \sim -3$ as well as the weakest line (313.1) of the Be II doublet. Note, that $S/N$ for the O I IR triplet was lower than 500 because these lines lie at the edges of the spectral orders.

The observational data were processed to compensate for instrumental effects and were thus converted into a spectrum format, number of counts versus wavelength. Charge-coupled device (CCD) detectors add a bias when reading the signal. Their response to the signal is in general different at different
Figure 3.1: Observed spectra of the BeII UV doublet lines, the OI forbidden line and triplet lines for HD 4306 with [Fe/H]=-2.33.
pixels (detector units). To correct for that, flat-field exposures were regularly taken, and the observations minus bias were divided by these flat-fields. The quality of the resulting spectra is high, as can be observed in Fig. 3.1.

3.2 Stellar parameters and 1D-LTE model atmospheres

The formation of spectral lines depends on the properties of stellar atmospheres such as temperature and density. These properties can be modelled using model atmosphere codes once the fundamental stellar parameters are known: effective temperature \( T_{\text{eff}} \), surface gravity \( \log g \), metallicity \([\text{Fe/H}]\) and microturbulence \(\xi_{\text{micro}}\). These parameters determine the main properties of the stellar atmospheres. The effective temperature is the temperature of a black body whose emitted flux is the same as the total stellar flux. The effective temperature is thus in terms of the stellar luminosity \( L \) and the stellar radius \( R \),

\[
T_{\text{eff}} = \left( \frac{L}{4\pi \sigma R^2} \right)^{1/4}
\]

and the surface gravity in terms of stellar mass \( M \) and \( R \)

\[
\log g = \log \left( \frac{GM}{R^2} \right),
\]

\( \sigma \) is Stefan-Boltzmann’s radiation constant and \( G \) Newton’s gravitational constant. Our abundance determinations are based on \( T_{\text{eff}} \) estimates from colour index-\( T_{\text{eff}} \) calibrations, in particular the \((b - y)\)- and \((V - K)\)-\( T_{\text{eff}} \) calibrations in Alonso et al. (1999). A colour index is defined as the difference in photometric magnitude measured through two different pass bands, while the magnitude is a measure of the brightness of an astronomical object. Once \( T_{\text{eff}} \) was determined, the surface gravity could be estimated from the Hipparcos parallax (Perryman and ESA (1997)) and the visual magnitude \( V \) (see Eq. 3 in Nissen et al. (1997)). The stellar parameter determination becomes an iterative process when metallicity is derived from spectral synthesis as the \((b - y)\)- and \((V - K)\)-\( T_{\text{eff}} \) calibrations depend on metallicity. In the first approach, the metallicity was obtained from photometry but later on, when also \( T_{\text{eff}}, \log g \) and \( \xi_{\text{micro}} \) had been determined, new metallicity estimates were obtained from the analysis of 13 observed Fe II lines at different wavelengths (490.0-650.0 nm) in the programme star spectrum. The analysis was performed by comparison to the solar spectrum. The Fe II oscillator strengths were determined from the solar spectrum and were used in the stellar analysis performed with the same program as used for the Sun. Thus, the Fe analysis is strictly differential. Solar equivalent widths were taken from the published values of Nissen et al. (2002). The microturbulence is a parameter introduced by stellar spectroscopists to describe the line profile broadening and strengthening.
sumably due to turbulent motions at scales smaller than unity optical depths. We estimated the value of the microturbulence parameter by minimising the dispersion in the iron abundances derived from the 13 Fe II lines for each star. We ended up with effective temperatures between 4700 and 5400 K, typical logarithmic surface gravity values of the order of 3.0 (c.g.s. units) and values of metallicity covering a wide range \([-3.0, -1.5]\). The parallaxes of the programme stars suggested that they have distances in the range from \(10^2\) pc to \(10^3\) pc (1pc=3.2616 light years); large enough for the light of these objects to possibly be affected by interstellar dust extinction (so-called reddening). The photometry was corrected for reddening before it was used for determinations of stellar parameters.

In the 1970-1990’s, former and present members of the Stellar Atmosphere Group at Uppsala Astronomical Observatory developed a numerical method and a computer code (MARCS) (Gustafsson et al. (1975)) to model the photospheres of late-type stars. Several assumptions are made for these models: the stellar atmospheres are assumed to be in hydrostatic and in local thermodynamical equilibrium (LTE), they have either plane-parallel or spherical symmetry and the sum of the radiative and convective flux is constant throughout the atmosphere. Convection is described in these models by the mixing length theory Böhm-Vitense (1958). LTE conditions mean that the distributions of states of atoms and molecules are determined by the local properties of the gas, assuming the Maxwell-Boltzmann-Saha distributions to be relevant. We computed MARCS model atmospheres for the stellar parameters of the programme stars assuming the stars to have plane-parallel geometries.

3.3 Equivalent widths, synthetic spectra and abundances

Two different approaches may be used to determine stellar abundances from observed spectra with model atmospheres: analysis of equivalent widths or spectral synthesis. Both methods are based on the modelling of the formation of the spectral lines. An equivalent width is the area of the line normalised on the continuum flux, and its measurement gives a measure of the spectral line strength and thus of the stellar elemental abundance:

\[
W = \int_{\lambda_1}^{\lambda_2} \frac{F_c - F_\lambda}{F_c} d\lambda
\]

(3.3)

where \(F_c\) and \(F_\lambda\) are the continuum and monochromatic flux, respectively, and \(\lambda_1\) and \(\lambda_2\) are chosen on either side of the line.

The equivalent-width method may be applied for clean lines where the continuum may easily be located. When using this method it is not necessary to model the line broadening by large scale motions in the stellar atmospheres,
Table 3.1: Lines used for abundance determinations and their laboratory wavelengths, excitation potential, logarithm of the product of the statistical weight of the lower line level and the oscillator strength, statistical weight of the upper level and reference from where the data were taken. (1) Smith et al. (1993), (2) Primas et al. (1997), (3) Nissen et al. (2002) and (4) Gillis et al. (2001).

<table>
<thead>
<tr>
<th>Species</th>
<th>λ [nm]</th>
<th>χ [eV]</th>
<th>log f</th>
<th>g_u</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li I</td>
<td>670.78</td>
<td>0.00</td>
<td>0.17</td>
<td>4.00</td>
<td>(1)</td>
</tr>
<tr>
<td>Be II</td>
<td>313.11</td>
<td>0.00</td>
<td>-0.47</td>
<td>2.00</td>
<td>(2)</td>
</tr>
<tr>
<td>Be II</td>
<td>313.04</td>
<td>0.00</td>
<td>-0.47</td>
<td>2.00</td>
<td>(2)</td>
</tr>
<tr>
<td>O I</td>
<td>777.19</td>
<td>9.14</td>
<td>0.37</td>
<td>7.00</td>
<td>(3)</td>
</tr>
<tr>
<td>O I</td>
<td>777.42</td>
<td>9.14</td>
<td>0.00</td>
<td>3.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>499.33</td>
<td>2.81</td>
<td>-3.54</td>
<td>8.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>510.07</td>
<td>2.81</td>
<td>-4.19</td>
<td>8.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>519.76</td>
<td>3.23</td>
<td>-2.28</td>
<td>6.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>523.46</td>
<td>3.22</td>
<td>-2.20</td>
<td>6.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>532.55</td>
<td>3.22</td>
<td>-2.20</td>
<td>6.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>541.41</td>
<td>3.22</td>
<td>-3.80</td>
<td>8.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>542.53</td>
<td>3.20</td>
<td>-3.42</td>
<td>10.00</td>
<td>(3)</td>
</tr>
<tr>
<td>Fe II</td>
<td>614.92</td>
<td>3.89</td>
<td>-2.77</td>
<td>2.00</td>
<td>(3)</td>
</tr>
</tbody>
</table>

such as macroturbulence or rotation (see e.g. Gray (1992)). The spectral-synthesis method consists on fitting observed line profiles or spectra with synthetic spectra. It is recommended for lines in the UV, since in this wavelength region blends are a major problem as is the determination of the continuum level. We made use of spectral synthesis for the Be II lines and seven OH UV lines with wavelengths ranging between 310.3 and 326.2 nm. For the rest of the lines we preferred the equivalent-width method, as in our target stars the lines are unperturbed.

Programs from the Uppsala model atmosphere package were used to model the formation of the lines of interest. The equation of radiative transfer was solved under the assumption of plane-parallel geometries and LTE conditions.
giving for the emergent flux at the stellar surface \( (F^+_\nu) \)

\[
F^+_\nu = 2\pi \int_0^1 \int_0^D \mu S_\nu e^{-\tau_\nu} d\tau_\nu d\mu
\]  

(3.4)

with \( \mu \) denoting the cosine of the polar angle (\( \cos \theta \)). \( S_\nu \) is the source function which is the ratio between the monochromatic emissivity \( (\eta_\nu) \) and extinction coefficient \( (\alpha_\nu) \). The source function used in our LTE analysis is

\[
S_\nu = \frac{\kappa_\nu}{\alpha_\nu} B_\nu + \frac{\sigma_\nu}{\alpha_\nu} J_\nu
\]  

(3.5)

where \( \kappa_\nu \) and \( \sigma_\nu \) are the absorption and scattering coefficients, respectively, and \( J_\nu \) is the mean intensity. When scattering is insignificant, the source function approaches the Planck function \( (B_\nu) \) which is a function of only temperature and frequency. This is, however, not the case in the UV region of our spectra, where Rayleigh scattering by hydrogen atoms is important. The optical depth \( (\tau_\nu) \) is the integral of the extinction coefficient \( (\alpha_\nu) \) along the ray

\[
\tau_\nu(z_0) = \int_{z_0}^D \alpha_\nu dz/\mu.
\]  

(3.6)

In strong spectral lines, the extinction coefficient is roughly proportional to the population of the lower level of the considered transition as well as to the transition probability. These populations are determined by the Saha-Boltzmann distribution. The atomic and molecular data used for the lines of interest are shown in Table 3.1. Note that in the UV, it was necessary to synthesise additional blending lines. The information on these other lines was obtained from the Vienna Atomic Line Database (VA L D) Piskunov et al. (1995) and from previous work by Francesca Primas. Line profiles are affected by microscopic collisions and stellar motions on either small (microturbulence) or large (macroturbulence) scales. The modelling of these broadenings was based on Gaussian and Voigt profiles with appropriate damping constants. Also, Gaussians provided good descriptions of the instrumental line broadening. The widths of these Gaussians were determined from the spectral resolution of the observations; the nominal resolving power \( (R = \lambda / d\lambda) \) at the center of the order and for the instrumental configuration used in the UV is \( \sim 45000 \), and \( \sim 60000 \) in the optical-near-IR.

In Table 3.2 the Li, Be and O abundances \( (A(X)) \) are summarised as determined from different indicators as well as the stellar parameters adopted for the programme stars. If several lines are used for the one species in Table 3.2, a mean value is given for the abundance. All abundances given in the table were determined by us; in the solar case only the [O I]-based oxygen and iron

\[ A(X) = \log \varepsilon(X) + 12. \]
Table 3.2: Stellar parameters and logarithmic abundances for the programme stars and for the Sun.

<table>
<thead>
<tr>
<th>Star</th>
<th>$T_{\text{eff}}$ [K]</th>
<th>log $g$ [cgs]</th>
<th>[Fe/H] [dex]</th>
<th>$A$(Li) [dex]</th>
<th>$A$(Be) [dex]</th>
<th>$A$(O) [dex]</th>
<th>$A$(O) [dex]</th>
<th>$A$(O) [dex]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sun</td>
<td>5780</td>
<td>4.44</td>
<td>0.00</td>
<td>8.74</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HD 4306</td>
<td>4990</td>
<td>3.04</td>
<td>−2.33</td>
<td>0.97</td>
<td>−1.84</td>
<td>7.14</td>
<td>7.40</td>
<td>6.68</td>
</tr>
<tr>
<td>HD 26169</td>
<td>4972</td>
<td>2.49</td>
<td>−2.28</td>
<td>0.91</td>
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abundances were determined.

A different combination of stellar parameters may result in different abundances. The sensitivity of abundances to errors in stellar parameters were investigated by perturbing the parameter values in Table 3.2 by 100 K, about 0.3-0.4 in \( \log g \) and 0.1 dex in [Fe/H] and deriving new abundances. The results suggest that accurate \( T_{\text{eff}} \) are necessary for determining accurate abundances, especially for abundances based on the Li I line, the seven OH UV and O I IR lines. Typical errors due to uncertainties in \( T_{\text{eff}} \) may amount to 0.1-0.2 dex. On the other hand, Be and Fe abundances are almost insensitive to the errors in \( T_{\text{eff}} \). Abundance determinations may also be sensitive to uncertainties in gravities. For the Be, O and Fe abundances they may amount to 0.1-0.2 dex. The metallicity uncertainties are less significant. Observational errors, either associated with spectrum noise or continuum level localization in spite of our high quality spectra are also important, in particular for very weak lines such as for the most metal-poor stars.

3.4 Abundance corrections for 1D-LTE abundances

Our abundance determinations were based on two important assumptions: plane-parallel geometries and LTE conditions. For certain spectral features inhomogeneities in stellar atmospheres as well as line formation out of LTE may affect the results. The modelling of these lines will thus require a detailed description of the radiation and its interaction with the atoms (NLTE) and more sophisticated model atmospheres; e.g. 3D-hydrodynamical models. 3D-NLTE models are still not available. Studies of spectral line formation under NLTE is not a new research field; schematic studies have been made since the 1950’s. However, realistic NLTE calculations require a lot of accurate atomic/molecular data and efficient algorithms. Adequate data are still missing for many atoms and molecules and NLTE line formation still remains to be investigated for many species.

Abundance studies in late-type stars using 3D model atmospheres have a more recent history, mainly because of the computer limitations. This is an area where systematic exploration started only during the last two decades. For the surface layers of the atmospheres of metal-poor main sequence stars, 3D models show average temperatures lower than 1D models. Some of the indicators in Table 3.1 are quite sensitive to the stellar temperature structure so they may be affected by the presence of inhomogeneities in stellar atmospheres. If this is the case, some of our abundances would suffer from systematic errors. The effects of such errors should be investigated when 3D models atmospheres are available with values of the stellar fundamental parameters typical of subgiants.
Line formation in NLTE is described in more detail in Sec. 6 where Paper III is discussed. Here, I just comment on the abundance corrections for NLTE effects on the abundance values in Table 3.2. All the corrections were computed with the same code, MULTI (Carlsson (1986)). However, only in the case of Be II and O I IR lines, specific NLTE computations were made for our programme stars. In the case of the Li I line, NLTE corrections were based on published results (Carlsson et al. (1994)). The abundance corrections for Li suggested that Li abundances are significantly affected by departures from LTE; they are always positive and their typical values are of the order of $+0.1$ dex. The NLTE abundance corrections to oxygen abundances based on the infrared triplet lines are always negative, about $-0.1$ dex. Corrections to the Be abundance may have different signs and cover a range from $-0.1$ to $+0.2$ dex, depending on the stellar parameters. No detailed NLTE calculations have been carried out for OH lines, although a very preliminary investigation was performed in Asplund and García Pérez (2001). Departures from LTE for our Fe II lines are expected to be small for the programme stars Nissen et al. (2002).
4 Oxygen debate (Paper I)

The common oxygen abundance indicators used for late-type stars are the near OH UV $\lambda \lambda^{2} v - X^{2} t$ electronic bands around 310.0 nm (OH UV), the forbidden O I lines at 630.0 and 636.4 nm ([O I]), the O I triplet lines at 777.1-5 (O I IR) and the OH IR vibration-rotation bands at 1.5-1.7 $\mu$m (OH IR). In general, different indicators are observed in stars of different stellar evolution phases. This is because the strengths of the lines depend on the temperatures and surface gravities of the stars. In spectra of metal-poor main-sequence stars, the [O I] lines become very weak and difficult to detect. Main-sequence (hydrogen core-burning) stars are in an evolutionary phase similar to that of the Sun. As these stars later evolve off the main-sequence they become giants (with a hydrogen burning-shell) and their stellar atmospheres get cooler. In the atmospheres of metal-poor giants, the high excitation O I IR lines (9 eV) get weaker as a consequence of this cooling, so [O I] lines are observed instead. Typical abundance results for metal-poor giants based on these lines are $[\text{O}/\text{Fe}] \sim 0.4$ (Barbuy (1988)) which seems to agree well with OH IR based results (Meléndez et al. (2001)). Abia and Rebolo (1989) determined oxygen abundances from O I IR in the spectra of metal-poor dwarfs. Their [O/Fe] results were much higher than +0.4 and it set in some way the stage for a vigorous debate on the oxygen abundances of Pop II stars which intensified when results based on OH UV lines for metal-poor dwarfs were published by Israeliian et al. (1998), Boesgaard et al. (1999b) and Israeliian et al. (2001). These results indicated significantly higher values of $[\text{O}/\text{Fe}]$ than +0.4 dex, which suggested a linearly increasing trend with decreasing metallicity behaviour difficult to explain by contemporary standard models of the Galactic chemical evolution. Further, there are reasons to believe that the indicators giving the high $[\text{O}/\text{Fe}]$ values may not be the optimal ones as discussed in e.g. Asplund and García Pérez (2001) and Nissen et al. (2002). This is because the oxygen abundances derived from them seem to be quite dependent on the structure of the stellar atmospheres which may be not adequately modelled. Molecular information for the OH lines is not very rich. The advent of 8m telescopes and highly efficient spectrographs made it possible to detect weak lines in spectra of low metallicity dwarfs Nissen et al. (2002). The forbidden line in dwarfs also suggested lower $[\text{O}/\text{Fe}]$ values than those derived from the OH lines. Nissen et al. (2002) also derived oxygen abundances from O I and
Figure 4.1: [O/Fe] estimates as a function of metallicity. Estimates based on different indicators are shown separately: [O I] 630.03 nm (top panel), O I IR 777.1-5 nm (middle panel) and OH UV around 310.0 nm (bottom panel).
the results were reasonably compatible with the values derived from the forbidden line. Our group, motivated by the results presented in Asplund and García Pérez (2001) and with the aim of clarifying why such divergent results appear, has carried out a more systematic study of these abundances in a sample of metal-poor subgiants \((-3.0 \leq [\text{Fe/H}] \leq -1.5)\). The parameters of these stars are optimal for detection of the [O I], O I IR and OH UV lines in their spectra. Their temperatures permitted us to detect the [O I] at 630.03 nm and O I IR lines at low metallicities. Besides, extrapolating results in Asplund and García Pérez (2001), one may guess that the oxygen abundances derived from OH UV lines for cool stars are less plagued by systematic errors than those of hotter stars.

In Paper I we have investigated the differences in oxygen abundances as estimated from different indicators observed in the same sample of metal-poor stars. One should note that OH UV lines represent a main oxygen abundance indicator at low metallicity for dwarfs which indeed demands a good understanding of their formation and the underlying molecular physics. For our stars oxygen abundance estimates based on O I IR lines give on average higher values than those derived from the [O I] lines while OH-based estimates give lower values. The mean differences between O I IR- and [O I]-based estimates (estimates based on O I IR were corrected for LTE departures) and OH UV- and [O I]-based estimates are \(0.19 \pm 0.22\) and \(-0.09 \pm 0.25\), respectively. Obviously, the scatter is not negligible.

One way to explore the cause of these differences is to investigate the effect of changing the stellar parameters. Oxygen abundances based on the different indicators react differently to changes in \(T_{\text{eff}}\). A \(T_{\text{eff}}\)-scale hotter by 100 K than the assumed scale will reduce the mean differences to approximately 0.05 (both mean differences now being positive). Abundances determined from the atomic lines are sensitive to surface gravity in the same way and by similar amounts so differences between them are not reduced when changing the adopted surface gravity. However, molecular lines and atomic lines react in opposite direction to these changes so abundance estimates based on OH lines increase with decreasing surface gravities. It is even possible to reach values higher than the values based on O I lines. The reddening effects may not have been completely removed from the programme star observations which would translate into too low values for the \(T_{\text{eff}}\) as determined from photometry. When higher values were assumed for the redenning this usually improved the agreement between the [O I] and O I IR abundance indicators but not between [O I] and OH indicators. In both cases the scatter in the differences remained quite significant as well as the dependence of the differences with \(T_{\text{eff}}\).

Our iron abundance determinations are relatively insensitive to effective temperature changes of the order of 100 K. Unfortunately they are sensitive
to surface gravity changes; however, the sensitivity is such that it is negligible when considering \([O/Fe]\) from \([O\,i]\) and \(O\,i\) IR. Uncertainties in the gravities are added when estimating \([O/Fe]\) from molecular lines. The result of this and of the higher sensitivity to stellar parameters is that the \([O/Fe]\) uncertainties for oxygen abundances based on the molecular lines are the highest (0.30 dex) while uncertainties for the abundances based on the atomic lines are lower (~ 0.15 dex).

Molecular and high excitation atomic lines like the \(O\,i\) IR are quite sensitive to the temperature structure so they may require detailed model atmospheres and radiative transfer in order to accurately describe their formation (3D-LTE model atmospheres, 3D-NLTE model atmospheres, 3D-NLTE line formation).

For these reasons, we have preferred \([O\,i]\) over the other indicators as a basis for discussion of the chemical evolution of oxygen at low metallicity. The differences between the different indicators also suggest this. It is also true that iron abundances may be affected by inaccuracies of the stellar model atmosphere or the radiative transfer which could be canceled out when combining with oxygen abundances. For the moment and as long as 3D-LTE model atmospheres are unavailable with the programme stellar parameters, we consider the \(O\,i\) forbidden line as the best oxygen abundance indicator.

Fitting \([O/Fe]\) versus \([Fe/H]\), we found a linear relation between \([Fe/H] = -3.00\) and \(-1.00\) of the type \([O/Fe] = -0.09(\pm 0.08)[Fe/H] + 0.36(\pm 0.15)\) which is in agreement with the previous study of Nissen et al. (2002) using the same indicator. However the slope of this trend is much smaller than the slope of the linear trends in Israelian et al. (1998); Boesgaard et al. (1999b); Israeli et al. (2001) which are based on results from a set of OH UV lines. And here comes the surprising result of our work: our present \([O/Fe]\) results based on OH lines lie below the trend found in previous studies based on the same indicator but for hotter stars closer to the main-sequence. Our OH-based trend is almost flat \([O/Fe] = -0.05(\pm 0.18)[Fe/H] + 0.38(\pm 0.40)\). If this discrepancy is caused by 3D-NLTE effects, the differences seen when comparing previous results with our result may suggest that these effects are smaller in subgiants than in dwarfs. Different stellar parameter scales in the studies may also be the reason for such discrepancies. The results for the stars with the highest effective temperatures in our observed sample lie close to previous results. According to Galactic chemical models in Chiappini et al. (2003) a small increase in \([O/Fe]\) when decreasing metallicity should be expected for stars at our metallicities. The supernova yields of oxygen depend on the stellar metallicity. The slope of the \(O\,i\) IR-based \([O/Fe]\)-vs-\([Fe/H]\) trend is much more pronounced \([O/Fe] = -0.40(\pm 0.11)[Fe/H] - 0.14(\pm 0.22)\) than the slopes of the other two trends based on the other criteria explored here and is also in agreement with results in Nissen et al. (2002). Oxygen-over-iron abundances versus metallicity are shown in Fig. 4. In the case of abundances
from the O I triplet lines, NLTE values are employed.
The processes mixing the light elements in stellar surface layers are still not fully understood. A simple mixing mechanism is convection described by the mixing length theory, the so-called standard mixing process (Deliyannis et al. (1990)). Pre-main-sequence stars of low mass are mostly convective but as they later evolve towards the main sequence, they develop radiative interiors. Thus stars are expected to deplete light elements during the pre-main-sequence but little or nothing at all during the main sequence because of the significant reduction in the depth of the surface convection zone. However, observations of main-sequence stars with $T_{\text{eff}} \sim 7000$ suggest that their Li and Be contents have been depleted. Boesgaard and Tripicco (1986) and Deliyannis et al. (1998) found that K stars in the Hyades cluster show Li and Be abundances lower than e.g. G stars. Plotting Li abundances versus $T_{\text{eff}}$, they found a dip in Li abundance around 7000 K (the so-called Boesgaard-Tripicco Li dip) and later they observed a Be dip at about the same temperature. Further evidence of depletion during the main-sequence phase comes from observations of open clusters with different ages: the older the clusters the lower Li abundances they show.

Why is it so important to learn more about depletion? Li is produced in Big-Bang nucleosynthesis. In the 1980’s, Spite and Spite (1982) observed the Li $\lambda$ line in a sample of metal-poor stars of different $T_{\text{eff}}$. According to their abundance results, the stars seem to show a logarithmic content of lithium of 2.2 (on a scale with the content of H being 12.0) for a wide range of $T_{\text{eff}}$ around 6000 K, the so-called Spite Li-plateau. These results represented a big step forward in determining the value of the primordial lithium abundance and thus of the baryonic density $\eta$ of the Universe. However, the meteoritic Li abundance of 3.25 (Asplund et al. (2004)) is higher than this value. On the other hand, the solar photospheric value 1.05 (Asplund et al. (2004)) is lower, due to a depletion mechanism which is yet not fully understood. This suggests the possibility that the Spite plateau value is lowered from the cosmological level by depletion. According to standard mixing models convection on its own, if at all efficient, is not efficient enough to produce the large depletion from the meteoritic value to the solar photospheric value. Other mixing processes like diffusion, rotation induced processes, gravitational settling, radiative selective levitation as well as mass-loss have been invoked to explain depletions for
stars for which the standard mixing predicts depletion by wrong amounts or even nothing at all. However, the small amount of observed scatter in the Li abundances for stars on the Spite plateau is difficult to reconcile with theory which predicts that depletion should depend on stellar properties such as mass, rotation velocity, metallicity etc. $^7$Li is more stable than $^6$Li. Hence, detection of $^6$Li severely limits the amount of $^7$Li depletion (Smith et al. (1993, 1998)). Work on the detection of $^6$Li in metal-poor stars is in progress; however, its detection demands spectra of extremely high quality.

Be abundances on the other hand have been observed at low metallicity (Gilmore et al. (1992); Boesgaard et al. (1999a); Primas et al. (2000)). These observations suggest a relation between O and Be abundances, indicating that the Be abundance changes as the Galaxy evolves.

In Paper II we discuss mixing in subgiants on the basis of the derived Li and Be abundances results. These stars are on their way towards the red giant branch so their atmospheres are gradually expanding and cooling. As a consequence of this, their surface convection zones penetrate into layers where Li has been burnt earlier. When this happens, material poor in Li is mixed with the rest of the surface material by convection, so that Li is diluted. This also happens to Be, however the effect of the Be dilution is expected to be smaller because Be is less fragile than Li. The layer where Li survives burning is thinner than the Be layer.

Mixing models may be better constrained when not only Li but also Be abundances are added to the mixing picture. However, the requirement to detect the Be II resonance lines in metal-poor stars is higher than to detect Li I lines, not the least the weakest of the two (at 313.1 nm). The Be II line at 313.0 nm is stronger but is also problematic since it is severely blended. Detection of these lines in very metal-poor stars is thus a major challenge and even more so when dealing with subgiants which are expected to be depleted in these light elements. We succeeded, however, to detect the lines in most of the programme stars due to the good quality of our UVES spectra.

According to our abundance results, all the programme stars seem to show similar Li contents. The results do not suggest any obvious relation with metallicity. However, they seem to show some variation with $T_{\text{eff}}$. Standard mixing models predict more significant dilution as $T_{\text{eff}}$ decreases which is corroborated by our Li abundance results. For the Be abundances, as has also been found for main-sequence stars, logarithmic Be abundances seem to vary linearly with $[\text{O}/\text{H}]$. The relation is well described by a broken linear fit with slopes 0.46 and 0.90 and a break at $[\text{O}/\text{H}] = -2.1$. Comparing with values typical of main-sequence stars, the programme stars show much lower Li and Be abundances. For Li, we compare with Spite plateau values (Spite and Spite (1982); Ryan et al. (1999); Bonifacio and Molaro (1997)) and for Be and O with values determined for main-sequence stars by our group.
Table 5.1: Li and Be depletion factors for the programme stars, based on abundances in metal-poor main-sequence stars. Predictions based on Deliyannis et al. (1990) depletion isochrones are given in Col. 3 and Col. 5.

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<th>$D(\text{Li})$</th>
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Figure 5.1: Li and Be depletion factors as a function of effective temperature. Our estimates (filled circles) are compared with the predictions (open circles).
We estimated logarithmic dilution factors ($D(X) = A(X) - A_i(X)$ with $X = \text{Li, Be}$) from these typical main-sequence abundance values and NLTE values for the Li and Be abundances. In the case of Li, a value of $A_i(X) = 2.2$ was taken as representative of the Spite plateau while in the case of Be, $A_i(X)$ values were computed from a broken line at $[\text{O/H}] = -2.1$ and slopes of 0.55 and 1.25. This trend fits our own Be and O abundance results for main-sequence stars. One should point out that the scatter around that trend is not negligible. The observed dilution factors (see Table 5.1) are compared with standard predictions in Fig. 5. In general, the agreement between observations and predictions is good, Li is on average 0.07 dex less depleted than expected and Be is on average 0.2 dex more depleted. One should note that the scatter in the differences between observations and predictions is more significant for Be than for Li but also that the Be abundances are less accurate than Li abundances; the uncertainties associated with errors in the stellar parameters are of the same order as the scatter. The spectrum normalisation in the UV is not as accurate as the normalisation in the visible, and the choice of a too low continuum level would result in systematically low abundance estimates. These problems might explain the difference between observed and predicted depletion values. Putting aside this possibility, however, we could still reconcile Li and Be depletion by suggesting a higher initial Li abundance value, $A_i(\text{Li}) = 2.6$. A similar high value is suggested by the baryonic density obtained from the Wilkinson Microwave Anisotropy Probe data in combination with Big-Bang nucleosynthesis.
Bengt Strömgren was one of the pioneers in formulating the problem of radiative transfer under NLTE conditions. Under these conditions, the radiative transfer equation and the equations of statistical equilibrium for the level populations of the species are coupled and usually require numerical methods to be solved. The solution to the radiative transfer in NLTE thus demands large scale calculations. In 1950’s and 60’s, Richard Thomas was one of the champions for the application of NLTE in spectral analysis, e.g. when estimating atmospheric abundances. In stellar interiors, LTE is generally a very good approximation. Stellar atmospheres are much colder and less dense than their interiors, making atomic and electronic collisions in the atmospheres therefore less frequent. The photons carry information on conditions where they were emitted as they travel in the atmosphere. They can travel quite far before they are absorbed and may be scattered on their way. The invent of computers facilitated NLTE computations. Numerical methods were quite improved in the 1960’s and 1970’s, in particular by Feautrier, Auer and Mihalas and experienced a renaissance in the 1980’s with the invention of approximate lambda iterations. The NLTE code used in this thesis is based on a method developed by two Swedes, Göran Scharmer and Mats Carlsson in the 1980’s (Scharmer and Carlsson (1985)).

When the radiation fields lose their local character and collisions are of less significance, level populations are not given any more by the local properties of the gas but by the radiation properties, especially by the mean intensity ($\bar{J}_\nu$). Under NLTE conditions, the radiative transfer equation and the equations of statistical equilibrium need to be solved simultaneously. The equation of statistical equilibrium for atomic level $i$ is

$$n_i \int (R_{ij'} + C_{ij'}) - \int n_{j'}(R_{j'i} + C_{j'i}) = 0 \quad (6.1)$$

with $R_{ij'}$ and $C_{ij'}$ the radiative and collisional rate, respectively, between the level $i$ and $j'$ and $n_i$ is the population of the level $i$. The sums are taken over $j'$. The departures from LTE depend on how important the radiative processes are relative to the collisions. Under the two-level-atom approximation, the source function for a bound-bound transition (line source function) is

$$S'_\nu = (1 - \varepsilon)J'_\nu + \varepsilon B'_\nu \quad (6.2)$$
with \( \varepsilon = \frac{C_{ul}}{C_{ul} + A_{ul}} \) \hspace{1cm} (6.3)

with \( (1 - \varepsilon) \) determining the importance of scattering. In Eq. 6.2, \( \bar{J}_\nu \) is the mean intensity integrated over the line profile and \( A_{ul} \) and \( C_{ul} \) are the Einstein spontaneous emission coefficient and collisional rate, respectively. NLTE effects depend mainly on departures of the mean intensity from the local Planck function values. A value of \( J_\nu / B_\nu \) different from unity may lead to several different effects, (see Bruls et al. (1992));

1. Over-ionization \( (J_\nu / B_\nu > 1.0) \)

2. Over-recombination \( (J_\nu / B_\nu < 1.0) \)

3. Photon pumping \( (J_\nu / B_\nu > 1.0) \)

4. Under-excitation \( (J_\nu / B_\nu < 1.0) \)

5. Photon loss \( (f_{lu}) \)

6. Scattering \( (\varepsilon < 1.0) \)

In general, \( J_\nu / B_\nu > 1.0 \) in the UV for metal-poor late-type stars (except for in strong lines) so that radiative bound-free and bound-bound transitions at wavelengths in this range produce over-ionization and over-excitation, respectively, with respect to LTE conditions. This over-excitation over-populates upper levels of the atom, the process is called pumping. For transitions in the IR wavelengths the opposite happens, \( J_\nu / B_\nu < 1.0 \), radiative bound-free and bound-bound transitions lead to over-recombination and under-excitation.

The strength of a bound-bound transition depends on the oscillator strength \( (f_{lu}) \); if the line is very strong, many photons will be absorbed which under certain conditions would not be re-emitted, with consequently less photons scattered. The result of this may be an over-population of the lower level of the transition. If spectral lines are formed under NLTE conditions, abundances determined from them will may be affected also by these departures (Carlsson et al. (1994); Kiselman and Carlsson (1996); Kiselman (2001); Zhao and Gehren (2000)).

In Paper III, I have investigated the departures from LTE for the Be II UV resonance lines at 313.0-1 nm which are frequently used in stellar abundance analysis (e.g. Boesgaard (1976); García López et al. (1995)). I have there calculated abundance corrections to LTE values for a grid of MARCS model atmospheres. The stellar parameters for the grid were those given in Table 6.1. The atomic model was made of 71 levels: 51 of neutral Be, 19 of ionized
Be and one of twice ionized Be. The number of bound-bound transitions included were 243 and the number of bound-free transitions 70. The main NLTE effects found in the formation of the Be II UV resonance lines are over-ionization and over-excitation. In the first part of the paper, I identified the main NLTE processes producing such departures in a model atmosphere of effective temperature 5500 K, logarithmic surface gravity 4.00 (cgs), metallicity $-1.00$ and beryllium abundance $A(\text{Be}) = 0.50$. The over-ionization was mainly produced by UV bound-bound transitions in the lower part of the term diagram which led to over-population of high energy levels ($\sim 8$eV) of Be I, i.e. photon pumping. A few bound-bound transitions in the upper part of Be I were also important for the NLTE effects. Exactly how Be I then is ionized, whether by collisions or radiative transitions, has a minor effect on the over-ionization. The main bound-free transitions correspond to UV transitions from the lower part of the term diagram and a few IR transitions from high energy levels of Be I. The over-excitation is the result of the departures of the line source function from the local Planckian value $J_\nu/B_\nu$. The lower level of the Be II lines under study is the ground state of Be II. On one side, these lines are expected to be stronger as a consequence of the over-ionization. On the other side, the effect of over-excitation is to decrease the strength of the lines. Stronger lines require lower abundances than in LTE to reproduce LTE equivalent widths, while weaker lines require higher abundances. The over-population of the lower level of the lines increased the line optical depth which produced a shift outwards in the line formation depths. As a result of these opposite effects, abundance corrections to the LTE values for a given stellar parameter combination may vanish as a result of a cancellation between the effects even if the lines were formed under NLTE conditions. Collision rates, mean intensities, line strengths, ionization degree etc. change with stellar parameters so variations of NLTE abundance corrections are expected with stellar parameters. It is not trivial to predict the changes of over-ionization and over-excitation with stellar parameter changes because the cancellation effects vary as discussed in detail in Paper III. In general, over-ionization dominates at lower temperatures while over-excitation does so at higher temperatures. As the metallicity increases, photon-suction plays a major role while over-excitation and over-ionization lose significance. This
Figure 6.1: Variations of NLTE abundance corrections with stellar parameters for the BeII line at 313.0 nm. The top panel shows the results for log \( g \) = 2.5 while the middle and bottom panels correspond to log \( g \) = 3.5 and log \( g \) = 4.5, respectively. In each panel, the corrections are plotted versus metallicity with different symbols connected by a solid line denoting corrections at different values of temperature: 4500 K (diamonds), 5000 K (triangles), 5500 K (squares), 6000 K (crosses) and 6500 K (circles).
leads to almost negligible abundance corrections at solar metallicity. As the gravity increases, the over-ionization seems to take over so that the abundance corrections become lower and more negative. In Fig. 6, logarithmic abundance corrections are plotted versus metallicity for different values of $T_{\text{eff}}$ and $\log g$. NLTE corrections vary between 0.15 dex and -0.2 dex.
7 Future prospects

This thesis represents just the beginning of a project to determine accurate stellar abundances. These determinations are based so far on 1D-modelling of stellar atmospheres. Even in a 1D-modelling context, still there are several aspects of the abundance determinations that could be improved. One example is the effective temperature determinations; methods to determine $T_{\text{eff}}$ which are preferably reddening independent such as the hydrogen lines using sophisticated theory to model their broadening should be explored. We believe that 3D-modelling of the line in addition to line formation out of LTE would constitute an advance in the understanding of the nature of the contradictory results on oxygen abundances. For the moment, abundance results with 3D model atmospheres of main-sequence stars are quite promising.

This thesis confirms that subgiants are good targets to detect several indicators for oxygen abundances and the light element abundances of these stars are good indicators of mixing process acting in stellar atmospheres. These stars have the advantage of being more luminous than dwarfs and thus easier to observe. As a first thought, one may think that to extend this study to other subgiants will not contribute with anything new on the oxygen debate because our results based on the different features remained irreconciled. However, our oxygen abundance results based on OH lines are quite odd with respect to results for main-sequence stars, in the sense that our oxygen abundances are much lower. Oxygen abundances based on OH lines in dwarfs intensified the oxygen debate, therefore it may be worth to explore OH lines in a different sample of subgiants. Much more can be said about dilution if the observed sample is extended, especially where Be is concerned. The literature is not very extensive regarding Be abundances at low metallicity, hence it is highly recommend to extend the observations to more subgiants. We believe our Be results will attract the attention of theoreticians providing Be dilution predictions in the future to confront our dilution estimates.

The identification and understanding of the main processes taking part in the formation of spectral lines are of significant importance for accurate abundance determinations. The identification of these processes may contribute to reduce significantly the atomic model to a few levels and transitions which would result in less costly computations and for example facilitate 3D NLTE calculations. Work on hydrogen collisions is in progress, once specific cross-sections for atoms other than hydrogen or lithium are available, line formation
of atoms already studied should be revised. Studies of line formation can be extended to other atoms as well as to 3D model atmospheres.
I have been blessed with so many good friends, nice work colleagues, excellent collaborators and even better supervisors, that I will need more than a few pages to thank all of you. However, I believe that everyone of you who will probably read these acknowledgements but not see your names written know that in one or another way, you are part of this; here my more sincere gratitude.

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If I will have very good memories of my years as a PhD student in Uppsala it is because of the Atmosphere group. Both former and present members have created such a nice working atmosphere that from now on it will be not easy to satisfy my demands. I owe these good memories also to a former member of the Galaxy group, Eva.

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To my beloved brother and mother. You are so generous that you encouraged me to fly when you more needed me close by, I will never forget this. I feel very proud of being your sister and your daughter.

9 Summary in Swedish

Om förekomster av litium, beryllium och syre i metallfattiga stjärnor i Vintergatan

Genom att studera ljuset från stjärnorna kan vi lära oss mycket, inte bara om de enskilda stjärnorna, utan också om vad som har hänt innan de ens var födda. Om vi leder ljuset från stjärnorna igenom ett prisma får vi ett spektrum som talar om för oss vilka ämnen som finns i stjärnan. Har vi en modell för hur ljuset påverkats av att ha färdats genom stjärnans atmosfär kan vi också bestämma halten de olika grundämnen som finns i stjärnan. Dessa halter är under den större delen av stjärnans liv desamma som grundämneshalterna i gasen som stjärnan en gång bildades av. Därför kan vi, genom stjärnors kemiska sammansättning få en inblick i gasens sammansättning nära Big Bang för ungefär 13.5 miljarder år sedan. Vi kan också lära oss om hur vår Vintergatas bildades och om tidigare generationers stjärnors bidrag till förekomsten av olika grundämnen.

Den forskning som beskrivs i denna avhandling har dels handlat om att förbättra metoderna för hur information utvinns ur stjärnspektra, och dels om att observera några av de äldsta stjärnorna i vår galax, Vintergatan, och bestämma kemiska förekomster av litium, beryllium och syre i dessa stjärnor för att på så vis lära mer om dessa ämnes ursprung. Litium och beryllium förstörs dessutom i stjärnorna, så för att bestämma halten av dessa ämnen i gasen stjärnan bildades av, måste man ha en modell för hur mycket som förstörts under stjärnans livstid. De stjärnor som observerats för detta avhandlingsarbete är alla subjättar, dvs stjärnor i ett senare utvecklingsstadium än solen, vilket innebär att stjärnans atmosfär kan ha förörent av ämnen som producerats i stjärnans inre. Med hjälp av datormodeller för en stjärnas utveckling kan man beräkna hur mycket av olika grundämnen som producerats eller förstörts av stjärnan själv och hur dess atmosfärisk kemiska sammansättning har förändrats. Det finns vissa osäkerheter i dessa datormodeller bl.a. på grund av vår bristande förståelse för hur blandningsprocesser mellan ämnen från olika djup i stjärnan (som konvektion) fungerar. Då kan man använda de observationellt bestämda ämnesförekomsterna för att förbättra modellerna. En sådan observationell studie presenteras i denna avhandling (Artikel II).
Grundämnenas ursprung

Den kemiska sammansättningen av stjärnors atmosfärer härstammar från de grundämnen som bildades i samband med Big Bang och från kärnförbränning i tidigare stjärngenerationer eventuellt tillsammans med restprodukter av stjärnans egna fusionsreaktioner.


Olika stjärnor producerar olika mycket av de olika grundämnen, mest beroende på hur tung stjärnan är. Tunga stjärnor (stjärnor med större massa än ca åtta gånger solens massa) exploderar till slut som en supernova av typ II. De är storproducerare av ämnen såsom syre. Lättare stjärnor som solen dominerar kanske produktionen av kol i Universum liksom av ungefär hälften av alla grundämnen tyngre än järn. Den största delen av det järn som finns i kosmos idag härstammar från supernovor av typ Ia. I dessa sprängs en vit dvärg som nätt en kritisk massa sönder, förmodligen på grund av den samlad på sig för mycket massa från en kompanjonstjärna.

I samband med stjärsnamnernas död kastas dessa kärnprodukter ut i det interstellära mediet igen. De stjärnor som föds därefter vid ett senare tillfälle har på grund av denna anrikning en större andel tyngre grundämnen. Man kan därför anta att de mest metallfattiga stjärnorna idag också är de äldsta. Detta avhandlingsarbete har speciellt fokuserats på de gamla stjärnor som finns i Vintergatans halo (Artikel I och II).

Modellering av stjärnspektra

Grundämneshalten kan bestämmas från observerade stjärnspektra. För att göra detta måste man dock ha en realistisk modell av stjärnatmosfären, speciellt av hur temperatur, tryck och densitet varierar med djupet i atmosfären. Sedan 70-talet har Uppsala haft en ledande forskningsgrupp som konstruerat sådana modeller för stjärnor liknande solen, dvs stjärnor med en effektivtemperatur mindre än 8000 K. Utöver en modellatmosfär måste man också ha

**Artikel I - Syrehalter i metallfattiga subjättar, bestämda från [O I]-, O I- och OH-linjer**


1VLT - Very Large Telescope - är ett teleskop vid Europeiska sydobservatoriet i Chile.
Artikel II - Nedbrytning av litium och beryllium i subjättar

I Artikel II använder vi samma observationsmaterial som i Artikel I för att bestämma litium- och berylliumhalter. Dessa ämnen förstörs i stjärnor om de utsätts för tillräckligt höga temperaturer och deras halter kan därför fungera som en test av konvektion och andra blandningsprocesser i stjärnor. Alla våra subjättar visar tecken på en sådan minskning av Li- och Be-halterna. I stort stämmer minskningen relativt väl med de teoretiskt förutsagda värdena från standardmodeller av stjärnutveckling. Den observationella Li-minskningen är ungefär 20% lägre än den teoretiska medan för Be visar observationerna på ungefär 60% större förstörelse än förutsagt. Dessa skillnader kan möjligtvis förklaras med osäkerheter i kontinuumplacering för Be linjerna och en underskattad antagen ursprunglig Li-halt. Det senare är i linje med WMAP²-analysen av den kosmiska bakgrundsstrålningen, som tyder på en halt av Li producerat i Big Bang ungefär dubbelt så stor som den vi antagit utifrån analys av metallfattiga dvärgstjärnor.

Artikel III – Avvikelser från lokal termodynamisk jämvikt för bildandet av beryllium II UV resonanslinjer i stjärnor av soltyp

I den tredje artikeln presenterar vi en detaljerad teoretisk och numerisk studie över bildningen av Be II-resonanslinjerna vid 313 nm, vilka är de enda linjer som praktiskt kan användas för att bestämma Be-halten i soltypsstjärnor. För åändamålet har vi använt oss av planparallella MARCS modellatmosfärer. Våra beräkningar visar att linjebildningen inte kan beskrivas korrekt med LTE utan att både överjonisations och överexcitationseffekter finns i dessa stjärnor. Detta ger upphov till en överpopulation av både den undre och övre nivån i övergången. Båda effekterna drivs av strålningsterminal från UV som i solen har en medelintensitet som är större än den lokala Planck-funktionen. Korrekterna av haltbestämningen för avvikelsen från LTE har beräknats för ett stort nät av stjärnparametrar. På grund av att de två huvudeffekterna går i olika riktning när det gäller linjestyrka är korrektionerna relativt små, cirka ±40%. För solen kompenserar de två effekterna varandra nästan exakt medan i metallfattiga dvärgstjärnor är korrektionerna ±20%.

²WMAP - Wilkinson Microwave Anisotropy Probe, en satellit som mäter graden av anisotropi i den kosmiska mikrovågsbakgrunden.
Framtidsutsikter

En av de stora felkällorna i analysen av grundämneshalter i gamla stjärnor är
bestämningen av deras effektivtemperaturer. Därför är det viktigt, för framtida
undersökningar, att utveckla metoderna för effektivtemperaturbestämning,
t.ex. genom utnyttja temperaturberoendet hos vätelinjers breddning. Dessu-
tom behövs 3D-modeller av stjärnatmosfärer och spektrallinjer, där även av-
vikelser från lokal termodynamisk jämvikt tagits med i beräkningen. Sådana
modeller börjar nu bli tillgängliga. Att systematiskt kombinera sådana mod-
ellar med observationer av hög kvalitet är en framtida möjlighet av stor be-
tydelse vid detaljerad analys av stjärnspektra. Detta kommer att möjliggöra
väsentligt noggrannare bestämningar av grundämnesförekomster i stjärnor,
vilket förväntas ge ytterligare information om hur Vintergatan (och andra
galaxer) uppkommit, och om grundämnesuppbyggnaden i det unga Univer-
sum.
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