Experimental f-value and isotopic structure for the Ni I line blended with [OI] at 6300Å

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ABSTRACT

We have measured the oscillator strength of the Ni I line at 6300.34 Å, which is known to be blended with the forbidden [O I] λ6300 line, used for determination of the oxygen abundance in cool stars. We give also wavelengths of the two isotopic line components of ^{58}Ni and ^{60}Ni derived from the asymmetric laboratory line profile. These two line components of Ni I have to be considered when calculating a line profile of the 6300 Å feature observed in stellar and solar spectra. We also discuss the labelling of the energy levels involved in the Ni I line, as level mixing makes the theoretical predictions uncertain.

Subject headings: atomic data - Sun:abundances - stars:abundances

1. Introduction

Allende Prieto, Lambert & Asplund et al (2001, hereafter APLA) have recently reviewed the various ways to determine the oxygen abundance in the sun and other

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late-type stars and discussed the different problems connected with the spectral oxygen lines used. Stellar conditions limit the number of appropriate lines to a few allowed and forbidden lines of neutral oxygen (O I and [O I]) in the optical wavelength region and molecular OH in the UV and IR regions. A frequently used method to determine the oxygen abundance in cool stars and the sun is to use the forbidden [O I] line at 6300 Å, which is particularly studied and analysed in the solar spectrum by APLA. However, this line is associated with problems as it is blended with an Ni I in the solar spectrum. This was early pointed out by Lambert (1978). Since the [OI] line (6300.31 Å) and the blending Ni I line (6300.34 Å) appear as a totally unresolved feature in the solar spectrum APLA constructed a spectral profile from laboratory data (wavelengths and f-values) and compared with the observed solar feature. Three of four crucial atomic parameters are known to a satisfactory accuracy, viz. wavelength (Eriksson 1965) and f-value (Storey & Zeippen 2000) for the [OI] line and wavelength for the Ni I line (Litzén, Brault & Thorne 1993, hereafter LBT). APLA used a three- dimensional time-dependent hydrodynamical model to simulate the solar surface and applied the same technique as previously used by Asplund et al. (2000) in the determination of the solar iron abundance. They used three free parameters, the continuum level, the oxygen abundance and the product " gf-value of the Ni I line x nickel abundance, $gf\epsilon$(Ni)" to match the predicted and observed profiles. By inserting the adopted solar abundance of nickel from Grevesse and Sauval (1998) APLA derived an "astrophysical" log gf value of -2.31 for the Ni I line from the fitted value of $gf\epsilon$(Ni). We quote from the APLA paper: "The log gf for the Ni I line is uncertain. There are seemingly no laboratory measurements for this line".

We have now determined the gf-value of the Ni I line at 6300.34 Å by combining two-step laser-induced fluorescence (LIF) measurements of the radiative lifetime of the

upper level with branching fraction measurements using Fourier Transform Spectroscopy (FTS). We have also fitted two isotopic line components (^{58}Ni and ^{60}Ni) to the laboratory Ni I line and derived wavelengths and absolute intensities for both components. These two Ni isotopes account for 94% of the solar nickel abundance. We have reexamined the LS composition of the upper energy level of the Ni I transition, as it is severly mixed and has no clear LS signature. The level was discussed and reassigned in the extensive work on the Ni I spectrum by Litzén, Brault & Thorne (1993), and its identity has been further discussed by APLA. Adopting one or another of the "old" (4d e^3P_0) or the "new" ($4s^2\ ^1S_0$) assignment makes a difference in the f-value of a factor of 400 (a difference in log gf of 2.6) if we consult the Kurucz database, which is often used in abundance work using the spectrum synthesis technique. Thus, an experimental value of the oscillator strength will help in understanding the real LS composition of the energy level.

2. Atomic physics background

Since the Ni I line studied in this paper has a great influence on the determination of the oxygen abundance it deserves a special attention. Because of the level mixing there is a need for an experimental gf-value as well as a detailed study of the isotopic composition of the line. The effect of level mixing that makes calculated oscillator strengths very uncertain is a frequent problem in complex spectra. Very drastic cases may occur in modelling stellar spectra where a calculated spectral line, predicted by means of theoretical atomic data, totally disagrees with the observed feature.

To illustrate the level mixing in the present Ni I case we have included a small part of the Ni I term diagram in Fig. 1, showing the relevant energy levels involved in the

discussion as well as in the measurements. The upper level of the λ6300 Ni I line is located at 50276 cm^{-1} and the lower level is y^{3}D$^o_1$, which belongs to the odd parity 3d^{8}4s4p configuration. In the first analysis of the Ni I spectrum, Russell (1929) assigned the 50276 level to e$^3P_0$ of the even parity 3d^{9}4d configuration, which seemingly makes the transition to y$^3D^o_1$ a "two-electron jump". The appearance of such a transition can be explained by configuration interaction between 3d^{8}4s4p and 3d^{9}4p, making the line a participant of a regular 4p-4d transition. Theoretical calculations by Litzén et al. (1993) confirmed such a level mixing between y^{3}D$^o_1$ and z^{3}D$^o_1$ belonging to 3d^{8}4s4p and 3d^{9}4p, respectively.

In the NIST compilation of iron group elements (Corliss & Sugar 1981), issued before the LBT work, the 50276 level has been given the old label, 4d e$^3P_0$, suggested by Russell. However, the label of another level located at 51457 cm^{-1} was changed from 4d ^{1}S$_0$ to 4s^2 ^{1}S$_0$. This change is supported by Kurucz's calculations (2002) as the major eigenvector component is more than 90% of 4s^2 ^{1}S$_0$. The Kurucz calculation also confirms the "old" label of the 50276 level, as it was found to contain more than 95% e^{3}P$_0$. Strangely enough, the Cowan code calculations performed by LBT gave completely opposite results concerning these levels. The 50276 level contained a 90% component of 4s^2 ^{1}S$_0$, and the 51457 level was reassigned to the 4d configuration. LBT give the 4d labels in jK coupling notation, which is clearly justified by the level structure (see Fig. 3 in their paper).

According to Kurucz's calculations of log gf values both levels (50276 and 51457) have their strongest decay to z^{3}P$^o_1$ (see Fig. 1). However, the transitions to y^{3}D$^o_1$ differ by a factor 400 in the log gf values, which are -1.73 for the transition from 50276 and -4.38 from the 51457 level. The second strongest decay from the 51457 level is to

$z^1P_1^o$ according to Kurucz, but the corresponding line from 50276 should be very weak. However, the latter is observed in the laboratory spectrum by LBT. Thus, the 50276 level obviously has a significant singlet character, which might be difficult to predict with sufficient accuracy in the calculations. Therefore, we have measured the lifetime and the log gf-values, and analysed the isotopic structure.

3. Lifetime measurements

In the measurements of the radiative lifetime the 50276 level was populated by applying a two-step pulsed laser excitation with $z^3P_1^o$ as the intermediate level according to the scheme in Fig. 1. The radiative lifetime was derived by time-resolved observation of the fluorescence light released when the 50276 level decays to the lower odd levels. The experimental set-up was similar to the one described and illustrated in a recent paper by Nilsson et al. (2000). Free nickel atoms were created by laser ablation and excited to the level investigated by laser pulses from two Nd:YAG laser pumped dye lasers operating in the red spectral region. The wavelength of the first step excitation (3664 Å) was reached after frequency doubling and of the second step excitation (4811 Å) after Raman shifting in hydrogen gas. The two 10 ns pulses coincided in time and space during the interaction with the nickel atoms. Fluorescent light was detected using a monochromator and a fast photomultiplier. A digital transient recorder performed the data acquisition. The monochromator was set on one of the decay channels shown in Fig. 1. Most of the recordings were taken on the strong 4811 Å line. An average of 1000 single decay events was typically necessary for obtaining a good signal-to-noise ratio in the exponential decay curves. Thirty curves were recorded and the result for the lifetime of the 50276 level is 77±7 ns. The uncertainty of the lifetime is a combination of statistical and, although carefully checked, possible systematic errors. The standard

deviation of the 30 different measurements is less than 20% of the uncertainty.

4. Branching fractions and oscillator strengths

We have recorded the Ni I spectrum with the Lund UV Fourier Transform Spectrometer (FTS) and also extracted spectra from the Kitt Peak FTS database, previously used in the extensive study of the Ni spectrum by Litzén et al. (1993). All spectra are from hollow cathode lamps at various running conditions (pressure and DC current). The spectra have been intensity calibrated by means of branching ratios for internal argon lines (Whaling 1993), i.e. argon lines produced by the carrier gas in the nickel hollow cathode lamp. The branching fractions have been derived from the calibrated intensities of the spectral lines corresponding to the four decay channels indicated in Fig. 1.

Since the lower levels in all transitions studied have short radiative lifetimes there is no need for any corrections for self absorption in the light source. According to predictions and observations the transitions measured account for more than 99% of the decay from the 50276 level, and no residual branching fraction has to be considered. The total decay rate, given by the inverse value of the measured lifetime, has therefore been distributed among the four transitions in accordance with the experimental branching fractions. The results are given in Table 1. The uncertainties in the f-values are determined according to a procedure suggested by Sikström et al. (2002), and they include estimated errors in lifetime measurements, intensity measurements and the instrumental response function.

5. Discussion

There are some conclusions that can be drawn from Table I. Firstly, the "astrophysical" log gf value of the λ6300 line derived by ALPA in the fitting of the synthesized profile of the combined [OI] and Ni I lines to the observed solar line is closer to the present measurement than to the value given in the Kurucz database. The "astrophysical" log gf-value differs by 0.20 dex ($\approx 60\%$) from the new laboratory value, which has an uncertainty of about 0.05 dex (15%). Secondly, the triplet content of the level 50276 is overestimated in the calculations by Kurucz and perhaps underestimated in the calculations in LBT. Another strong evidence for a substantial contribution of the $4s^2\ ^1S_0$ state to the 50276 level is the isotope shift observed by LBT for the two strong lines $\lambda\lambda$4811,5780 in Table I, for which the the lower level belongs to the 4p configuration. Using Fabry-Perot interferometry Schroeder and Mack (1961) made a detailed study of the isotope shift in the lower configurations of Ni I. They found appreciable line shifts in transitions where the upper and lower configurations differ in the number of d-electrons. By calculating the normal mass shift and estimating the field shift they attributed the major part of these large shifts to specific mass shift. The absence of a significant isotopic shift in the 6300 Å line is thus consistent with a major

Table 1: Branching fractions (BF) and oscillator strengths (log gf) for Ni I lines from the level at 50276 cm^{-1} with a radiative lifetime of 77 ns.

Lower level	λ	BF	gA	log gf-value			unc.
	(Å)		(10^7 s^{-1})	this work	Kurucz	APLA	%
$3d^8 4s4p\ y^3D_1$	6300.341[a]	0.10	0.13	-2.11	-1.73	-2.31	14
$3d^9 4p\ z^1P_1$	5780.728	0.10	0.13	-2.18	-3.02		14
$3d^9 4p\ z^3D_1$	5162.913	0.02	0.03	-2.93	-1.93		28
$3d^9 4p\ z^3P_1$	4811.983	0.78	1.01	-1.45	-1.48		10

[a]Data for the isotopic line components: $\lambda(^{58}\mathrm{Ni})$=6300.335(1), $\lambda(^{60}\mathrm{Ni})$=6300.355(2); both have log gf=-2.11

contribution of $3d^8 4s^2\ ^1S_0$ to the 50276 level, as the configuration of the lower level, $3d^8 4s4p$, contains the same number of d-electrons. However, the observed profile of the laboratory 6300 Å line shows an asymmetry that could be due to isotopic structure. A small isotope shift would indicate a mixing of the upper state with a $3d^9 4d$ level or a mixing of the lower state with a $3d^9 4p$ level or a combination of the two. We have therefore examined the line more closely.

In Figure 2 we show the 6300 Å line as observed in the laboratory Fourier transform spectrum. We have fitted two isotopic line components to the observed feature, by assuming a solar ratio of 0.38 for the abundances of the ^{60}Ni and ^{58}Ni isotopes. We have neglected the other stable isotopes ^{61}Ni, ^{62}Ni, and ^{64}Ni as they contribute only 1.1 %, 3.6 % and 0.9 %, respectively. Furthermore, ^{61}Ni is smeared out by hyperfine structure. The wavelengths of the two isotopic components in the Ni I λ6300 line are 6300.335(1) for^{58}Ni and 6300.355(2) for^{60}Ni. The uncertainties of 1 and 2 mÅ respectively, include errors in the fitting of the line profile and calibration of the laboratory spectrum. The isotope shift of 20 mÅ is about the same as the distance of 25 mÅ between the [OI] line and the center of gravity (c.g.) wavelength for the Ni I line. Based on the present analysis we have derived new data for the c.g. of the line (previous values in parentheses are from LBT): σ= 15867.769 (.773) and λ=6300.341 (.339), and inserted the new c.g. wavelength in Table 1. The log gf value (-2.11) is the same for each isotopic line component.

The choice of LS label on the 50276 level is not evident, but it is quite clear that the 51457 level belongs to the 4d configuration. This level does not show any isotope shift in the transitions to 4p, which is characteristic for all transitions measured by LBT where there is no change in the number of d-electrons. Considering the apparent

labeling of the 51457 level and the observed isotope shift in the lines from the 50276 level the most appropriate label for the 50276 level is $4s^2\ ^1S_0$, as suggested by LBT. The observed isotope shift, which is of about the same size as for both $3d^9 4p$-$3d^8 4s^2$ and $3d^8 4s4p$-$3d^9 4d$ transitions, indicates level mixing but not the size of it. As pointed out by LBT an additional part of the problem may be caused by interaction with the unknown p^2 configuration, which contains both a $^1S_0$ and a $^3P_0$ level. Anyhow, the fact that the 50276 level contains a substantial amount of triplet character illustrates clearly the non-physical meaning and sometimes excessive ambition to assign an LS label to every energy level. However, it may be practical for book-keeping purposes to have a symbolic name on all energy levels.

6. Conclusion

The λ6300 [O I] line is one of the very few spectral features from which the oxygen abundance in the sun and cool stars (Allende Prieto et al. 2001) can be determined. The line is blended with an Ni I line, and a detailed study of the Ni I line at 6300.34 Å reveals an unresolved isotope structure. At least two isotopic line components, separated by 20 mÅ, have to be included when calculating a line profile to match the λ6300 feature in high resolution stellar and solar spectra. The log gf-values for the individual components should then be weighted by the relative abundances of the two isotopes.

We report in this paper on the wavelengths and log gf-values for the two major isotopic components of the Ni I line. We have measured the radiative lifetime of the upper level of the Ni I line using laser techniques and combined it with branching fractions to get the absolute transition probabilities. The branching fractions are derived from calibrated line intensities in a Fourier transform spectrum, which is also used to

disentangle the isotopic structure. The new experimental log gf value differ by 0.2 dex from the "astrophysical log gf value" derived by Allende Prieto et al (2001).

An apprporiate labelling of the upper level of the Ni I line has previously been discussed by Litzén et al. (1993). The additional information obtained in the present work, lifetime and isotopic structure, supports the label suggested in that paper.

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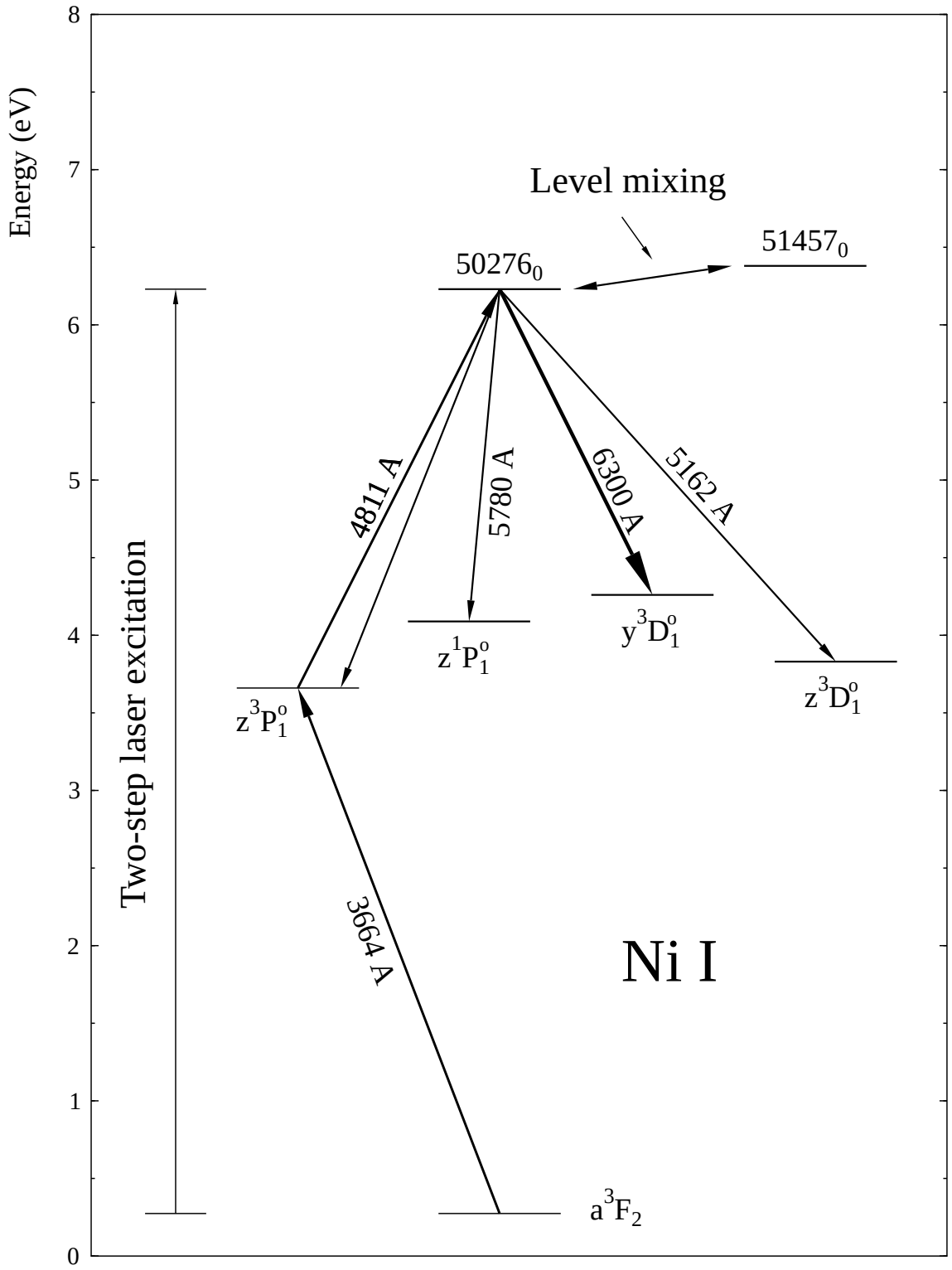

Fig. 1.— Partial level diagram of Ni I showing the levels and transitions discussed in this paper. The two-step excitation in the lifetime measurement is indicated to the left

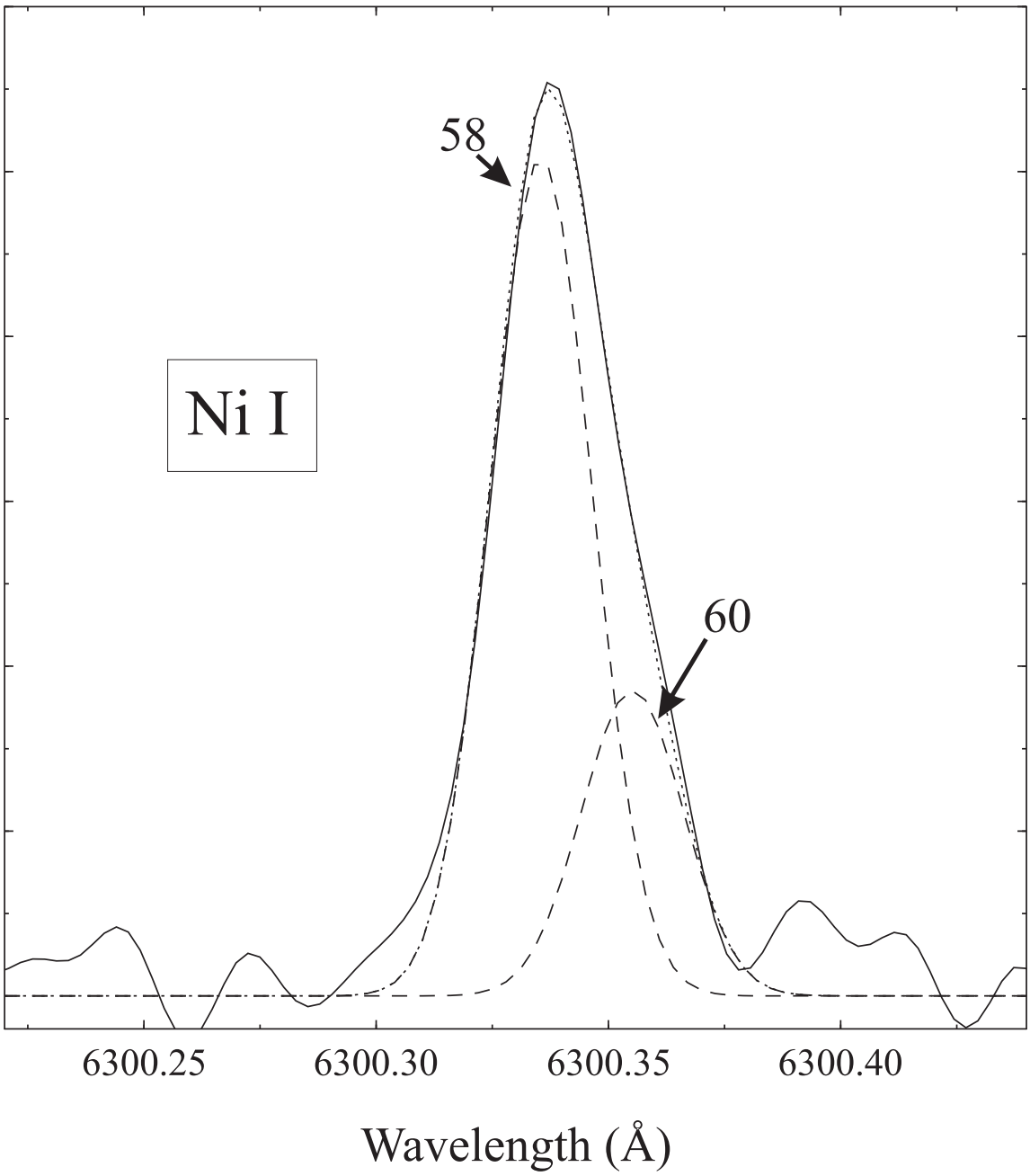

Fig. 2.— Laboratory FTS recording of the λ6300 line of Ni I with fitted line components for isotopes ^{58}Ni and ^{60}Ni.