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Investigation of the Hyperfine Structure of Atomic Niobuim (Nb I) Spectral Lines Based on the Lower Energy Levels at 22936, 23010, and 23048 cm^{-1}

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Abstract

The hyperfine (hf) structure constants of three atomic niobuim energy levels in the energy range around 23000 cm^{-1} (at 22936.90, 23010.58, and 23048.58 cm^{-1}) are known with only limited accuracy, and the constants of combining levels are sometimes even unknown. Thus we performed laser spectroscopic investigations in the wavelength range between 5600 and 6500 Å, and we excited altogether 16 transitions in which these lower levels are involved. Beside a more precise determination of the hf structure constants of the three lower levels (which were determined on several lines sharing a common upper level), these experiments led to the knowledge of the hf constants of nine levels with previously unknown constants. Beside these results, also the hf constants of 13 further energy levels are reported. For six of these levels, the constants were previously unknown.

Keywords

Niobium, Hyperfine Structure, Hyperfine Constants, Laser Spectroscopy

1. Introduction

Niobium (Z = 41) in its natural abundance has only one stable isotope. Its mass number is 93 and its nuclear spin quantum number is I = 9/2. It has a nuclear momentum of 6.1705 (3) μ_N and an electric quadrupole momentum of −0.32 (2) × 10^{-28} m^2 [1]. The electronic ground state configuration is [Kr] 4d^{4}5s and the ground state has the designation $^6D_{1/2}$. The Nb spectrum was investigated first by

J. Humphreys and W. F. Meggers [2]. Their energy values then were repeated in the famous tables of C. Moore [3]. Subsequently found energy levels were reported in refs. [4] [5] [6].

Investigations of the hyperfine (hf) structure of Nb spectral lines were performed by several authors [7] [8] [9] [10] [11]. Later on, studies were performed in a collaboration of groups in Berlin, Riga, and Istanbul [12]-[20]. Recently, the discovery of some new energy levels was reported [21]. This paper is a continuation of systematic studies of neutral niobium.

Despite all the efforts in the previous papers, the hf constants of a number of energy levels are not known with satisfying uncertainty or even unknown. Since the quadrupole moment of Nb is small, for most of the energy levels, the electric quadrupole constant B cannot be reliably determined from the experimentally observed hf patterns and is thus assumed to be zero. In such cases, the magnetic dipole constant A is describing the hf structure splitting sufficiently.

2. Experiment

The experimental procedure is the same as in the previous paper [21] but is also discussed e.g. in refs. [22] [23]. Free Nb atoms were produced in a hollow cathode discharge, cooled by liquid nitrogen. The discharge was operated with Ar at a pressure of ca. 0.5 mbar. After some minutes the sputtering process was fully developed and the discharge color changed to light blue which is characteristic for Nb. Then the discharge current was mainly carried by free Nb atoms, which are found in all excited states due to collision processes in the Nb-Ar-plasma.

Narrow-band laser light (line width ca. 1 MHz) was provided by means of a self-made ring dye laser, pumped by 532 nm laser light having a power of 5 W. The dye laser was operated with the dyes R6G (5540 - 6100 Å) and Kiton Red (5900 - 6500 Å). The output power was between 100 mW at the edges of the dye ranges and 500 mW at the peak of the corresponding range. The exciting laser light was intensity modulated by a mechanical chopper and sent through the hollow cathode discharge. The light emitted by the discharge was dispersed by means of a monochromator and detected on a suitable fluorescence line via a photomultiplier. The output signal of the multiplier was phase-sensitively amplified by means of a lock-in amplifier.

Due to laser excitation, the population of the lower level of the investigated transition is lowered and the population of the upper level is enhanced. The decay lines of the upper excited levels show thus an enhancement of their intensities when the laser light is on and its frequency is in resonance with an hf transition. This enhancement is detected as a laser-induced fluorescence (LIF) signal in phase with the modulated exciting light.

During the present investigations, we calculated possible transition wavelengths between the lower even levels of interest and upper odd energy levels in the wavelength range of our lasers using the program "Elements" [24] [25]. Then we set the laser wavelength to such a calculated value and searched for a LIF signal on a decay line of the odd upper level. Ca. 30 % of the experimental trials were successful. The corresponding wavelengths can be found in Table 1 and Table 2.

Table 1. Investigated levels and lines based on the lower levels at 22936, 23010 and 23048 cm^{-1}. tw this work. The line at 6435.52 Å can be fitted only assuming a relatively large value for B. Q is the qualtity of the fit (inverse proportional to the least quares error sum). The weighted mean values (printed in bold fonts) take into account the value of Q and the uncertainties of the hf constants.

Investigated level					Investigated line, combining level						Hf constants of the inv. level from ref.	
Energy (cm^{-1})	J	P	A (MHz)	B (MHz)	Wavel. (Å)	Energy (cm^{-1})	J	P	A (MHz)	Remark	A (MHz)	
Even												
22936.90	7/2	e	257.6 (20)		6444.89	39845.51	9/2	o	385.9 (20)*		266 (5)	[18]
23010.58	9/2	e	130.1 (20)		5938.38	39845.51	9/2	o	385.9 (20)		94 (10)	[18]
23048.58	11/2	e	84.7 (20)		5912.51	39845.51	9/2	o	385.9 (20)*		82 (4)	[18]
Odd												
38448.77	9/2	o	437.0 (30)		6444.89	22936.90	7/2	e	257.6 (20)*		390 (50)	[18]
38583.04	13/2	o	501.1 (20)	−135 (25)	6435.52	23048.58	11/2	e	84.7 (20)*			
39020.81	11/2	o	170.0 (30)		6244.28	23010.58	9/2	e	130.1 (20)*			
			345.1 (30)		6106.97	23010.58	9/2	e	130.1 (20)*	Q = 4		
39380.77	9/2	o	346.2 (30)		6121.18	23048.58	11/2	e	84.7 (20)*	Q = 2		
			345.6 (30)									
39426.84	7/2	o	516 (6)		6089.84	23010.58	9/2	e	130.1 (20)*			
39620.13	7/2	o	380.7 (20)		6018.97	23010.58	9/2	e	130.1 (20)*			
39845.51	9/2	o	385.9 (20)		5912.51	22936.90	7/2	e	257.6 (20)			
			374.1 (30)		5898.50	22936.90	7/2	e	257.6 (20)*	Q = 17		
39885.66	7/2	o	376.4 (30)		5924.26	23010.58	9/2	e	130.1 (20)*	Q = 6		
			374.7 (30)									
			402.4 (30)			23010.58	9/2	e	130.1 (20)*	Q = 2		
40003.00	11/2	o	405.2 (30)		5896.53	23048.58	11/2	e	84.7 (20)*	Q = 8		
			404.6 (30)									
			-		5856.05	22936.90	7/2	e	257.6 (20)*	Ok		
			320.0 (70)		5881.44	23010.58	9/2	e	130.1 (20)*	Q = 3		
40008.52	9/2	o	321.1 (30)		5894.61	23048.58	11/2	e	84.7 (20)*	Q = 8		
			320.8 (40)									
40421.93	9/2	o	324.0 (30)		5741.79	23010.58	9/2	e	130.1 (20)*			

*: value fixed in the fitting procedure; Ok: signal-to noise ratio too bad for data evaluation, but the observed hf pattern fits to the expected one.

3. The Line System Based on the Levels at 22936, 23010, and 23048 cm⁻¹

The hf structure constants A of these three even levels are given in ref. [18] to be as follows:

22936.90 cm^{-1}, J = 7/2: A = 266(6) MHz, at 8181.03 Å,

23010.58 cm^{-1}, J = 9/2: A = 94(10) MHz, at 8105.28 Å, and

23048.58 cm^{-1}, J = 11/2: A = 82(4) MHz, at 7945.65 Å.

Each value was determined on only one line in the near infrared region (wavelength mentioned above). All three lines have different upper energy levels.

Determination of the hf constants of these levels seemed to be desired since a larger number of transitions in the range of our lasers involve these three lower levels and upper levels with up to now unknown hf constants.

First we adjusted the laser wavelength subsequently to the calculated values. A LIF signal was found on altogether 13 transitions. Of special interest is the fact that now we can perform investigations on transitions where upper energy levels are excited from two or even all three interesting lower levels. The investigated line system is shown in **Figure 1**.

Table 2. Revised evaluation of lines from ref. [18] based on the lower levels at 22936, 23010 and 23048 cm^{-1}.

Investigated level				Investigated line, combining level					Hf constants of the inv. level from ref.	
Energy (cm^{-1})	J	P	A (MHz)	wavel. (Å)	Energy (cm^{-1})	J	P	A (MHz)	A (MHz)	
35156.94	9/2	o	509.7 (20)	8181.03	22,936.90	7/2	e	257.6 (20)*	510.0 (31)	[16]
35344.86	13/2	o	412.4 (20)	8105.03	23,010.58	9/2	e	130.1 (20)*	379.8 (500)**	[16]
35630.62	11/2	o	550.5 (20)	7945.65	23,048.58	11/2	e	84.7 (20)*	548 (4)***	[18]

* value fixed in the fitting procedure; ** in ref. [18], by mistake the A-value of the level at 35344 cm^{-1} is given as 510.0 (31) MHz. This value belongs to the level at 35156 cm^{-1}. But the fit was performed using correctly 379.8 MHz from ref. [16] (fixed in the fitting procedure); *** from evaluation of the same line assuming A (23048) = 82 MHz.

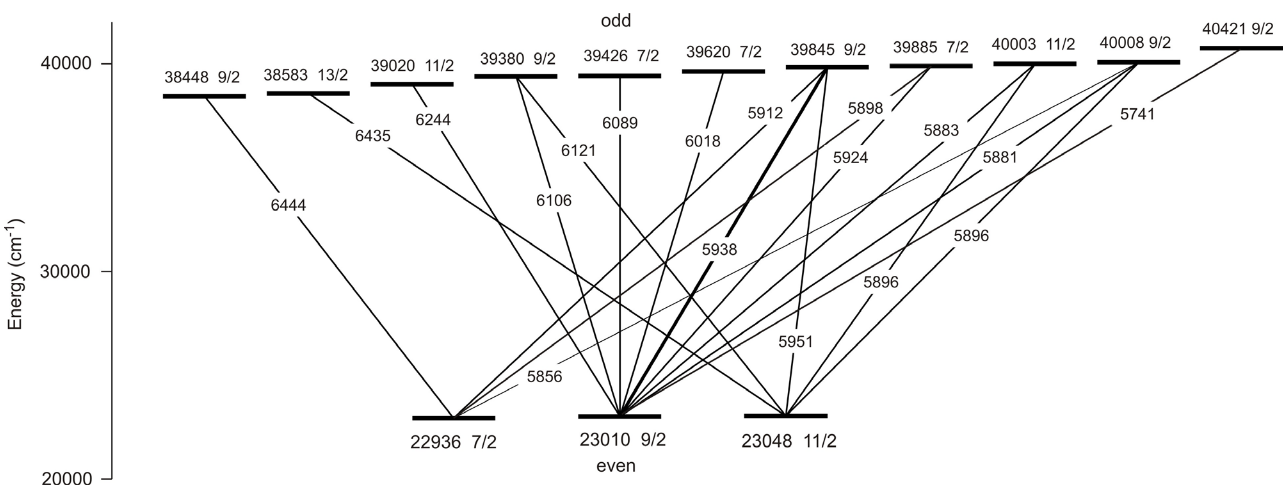

Figure 1. Investigated line system involving the lower energy levels at 22936, 23010, and 23048 cm^{-1}. Given is the level energy in cm^{-1} and the angular momentum. The transition wavelength is given in Å. Bold: key line at 5938 Å (see text). For reasons of clarity, no post decimal positions are given.

In principle, the hf constants of the involved energy levels can be found from a record of the hf pattern of an investigated line. However, in practice there are some limitations:

1) The signal-to noise-ratio (SNR) of the record must be sufficient. Especially it is important that the spectral position of less-intense hf components can be determined in order to find the hf constants of the involved energy levels without additional assumptions.

2) For Doppler-limited spectroscopy (as performed here) the distance between hf components to be fitted should be in the order of the FWHM of a single component or larger.

3) Sometimes the recorded pattern is rather sensitive to the difference of the A-factors of the combining levels than to their absolute values. Thus for the data evaluation the A-factor of one level must be known.

4) It may happen that the fit result is dependent on assumptions on the spectral line shape (which must be not the same for all components) and on the intensity ratios of neighboured components. This may be the case if the interaction of the laser light with the investigated atomic ensemble causes strong saturation effects due to optical pumping between the different hf sublevels.

These limitations made it difficult to determine precise values for the A constants of the lower levels, since the A-factors of nine combining upper levels were unknown and only one known, but with large uncertainty (A (38448) = 390 (50) MHz [14]).

Fortunately, among the three transitions to the upper energy level at 39845 cm^{-1} there was one line (at 5938 Å, transition to 23010 cm^{-1}) which allowed determining the A-factors of both involved levels reliably. For the determination of the hf constants we used the program "Fitter" as in various previous papers [26]. The recorded patterns show sufficient SNR, and the A-factors of upper and lower level combine in a way to establish relatively good resolved components or component groups. One of the recorded patterns is shown in **Figure 2**.

Indeed we were able to determine from this line the A-factor of the upper level and the lower level at 20310 cm^{-1}. From the lines at 5912 and 5951 Å we got then values for the other two lower levels at 22936 and 23048 cm^{-1}.

Next we investigated pairs of lines leading from two of the lower levels to a common upper level. Four pairs were available going to the upper levels at 39380, 39885, 40003, and 40008 cm^{-1}. Each line pattern was fitted independently, assuming the previously determined A-values for the lower levels to be fixed. The results for the constants of the upper levels agree with each other fairly (see **Table 1**). We give for the upper levels the weighted mean value of the results from these two determinations (bold figures in **Table 1**). For the last pair the SNR of the third line to the upper level 40008 cm^{-1} was too bad for a determination of the A-values, but the observed structure coincides nicely with the simulated pattern.

For the remaining five upper levels the A-factor was determined only on one line.

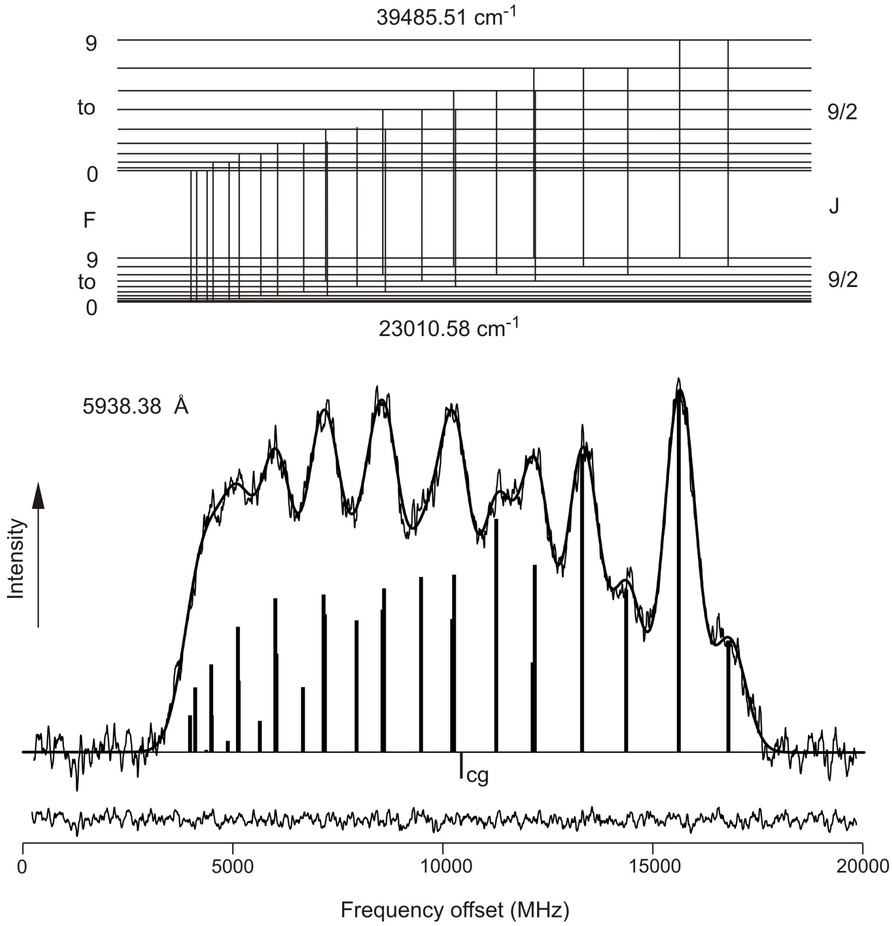

Figure 2. Recorded pattern of the line at 5938.38 Å (transition between 39845.51 cm^{-1}, J = 9/2, and 23010.58 cm^{-1}, J = 9/2). Closely neighbored hf components were coupled in the fit procedure to each other, but the intensities of the groups and the single standing components were treated as free parameters. The lower trace (difference of experimental and calculated curve multiplied by a factor of 0.5) shows no systematic deviations. cg marks the center of gravity.

All results are summarized in **Table 1**. In the first three columns energy, J and parity of the investigated level are given. Columns 4 and 5 give the hf constants A and B determined in this work. If no value for B is given, B was assumed to be zero. In column 6 the wavelength of the investigated line is given, and in columns 7 to 11 properties of the combining energy level. In the last Columns hf constants of the investigated level from literature are given, if available.

Since S.K. was co-author of ref. [18], we were interested in how the new results fit to the earlier data evaluation. Prof. Başar, Istanbul University, sent us the original data resulting from LIF investigations in the near infrared region. We fitted the hf patterns of the three relevant lines, this time using our hf constants of the lower energy levels as fixed parameters, without obtaining any contradictions. The results are given in **Table 2**.

When fitting the pattern of the line at 8181 Å we got for the A-factor of the level at 35156 cm^{-1} the value A = 509.7 (20) MHz, in complete agreement with

Table 3. Further investigated levels and lines. tw this work. The lines at 6427.55 and 5738.19 Å can be fitted only assuming relatively large valued for B. Mean values printed in bold fonts.

Investigated level					Investigated line, Combining level							hf constants of the inv. level from ref.		
Energy (cm^{-1})	J	P	A (MHz)	B (MHz)	wavel. (Å)	Energy (cm^{-1})	J	P	A (MHz)	B (MHz)	Ref.	A (MHz)	B (MHz)	
18332.04	11/2	e	3 (2)		5571.41	36275.77	11/2	o	545 (2)		tw	2.9 (6)	−94 (44)	[18]
19931.98	5/2	e	531.5 (10)		6422.69	35497.48	5/2	o	343.9 (10)*		[21]	529.0 (6)		[18]
20060.84	7/2	e	233.6 (15)		6476.30	35497.48	5/2	o	343.9 (10)*		[21]	244.5 (3)	2 (3)	[18]
26165.79	7/2	o	296.2 (5)	60 (10)	5838.61	9043.14	5/2	e	−407.8606 (4)*	35.060 (75)*	[8]	298.7 (13)	65 (20)	[18]
26713.32	3/2	o	112.3 (15)		6067.81	10237.51	5/2	e	295.6803 (6)*	36.501 (12)*	[8]	108.6 (4)	−19.6 (30)	[8]
28278.25	3/2	o	747.4 (10)	34 (10)	5903.80	11344.70	5/2	e	−639.3786 (7)*	−0.061 (92)*	[8]	748 (6)	14.7 (76)	[16]
29359.58	5/2	o	−15.5 (10)		5804.65	12136.86	7/2	e	502.4 (14)*		[5]			
32382.24	11/2	o	397.6 (10)	−230 (25)	6427.55	16828.52	9/2	e	744.4 (6)*	57 (12)	[18]	392.3 (91)		[17]
			11.1 (10)		6222.93	19034.71	7/2	e	477.6 (4)*	57 (40)	[18]			
35099.86	5/2	o	10.7 (10)		6436.90	19568.72	5/2	e	322.4 (2)*		[18]			
			10.9 (10)											
35178.82	7/2	o	558.2 (10)		6399.50	19556.91	9/2	e	112.7 (1)*	−12 (25)*	[18]			
35928.35	5/2	o	649.3 (15)		6110.94	19568.72	5/2	e	322.4 (2)*		[18]			
36275.77	11/2	o	545 (2)		5571.41	18332.04	11/2	e	3 (2)		tw			
36979.20	7/2	o	344.6 (10)	−114 (10)	5738.19	19556.91	9/2	e	112.7 (1)*	−12 (25)*	[18]			

* value fixed in the fitting procedure.

the value 510.0 (31) MHz from ref. [16]. For 35344 cm^{-1} we obtain A = 412.4 (20) MHz in agreement with 379.8 (500) MHz from ref. [16], but with much lower uncertainty. Finally, we obtain for level 35630 cm^{-1} A = 551.3 (20) MHz, close to the value in ref. [18], since the fixed value of A changed from 82 (4) to 84.7 (20) MHz only. These last values agree with each other within the given uncertainties.

4. Other Investigations

In the spectral range of our laser system we excited also some other transitions on which we were able to re-determine the hf constants of the involved energy levels or to determine—for altogether 6 levels—the constants for the first time. The results are shown in **Table 3**. The table is designed like **Table 1**.

5. Conclusion

In the present work, we focused mainly on the determination of more accurate hf constants of three levels around 23000 cm^{-1}. Indeed, using closed transition loops (see **Figure 1**), we were able to determine constants which allowed describing reliably and without contradiction, the hf patterns of the investigated lines. It was possible to determine the hf constants of nine energy levels for the first time and to lower the uncertainty of the A-factor of the level 38448 cm^{-1} from 50 to 3 MHz. Additionally, we investigated several lines in the treated spectral range. We could determine the A (and sometimes also B) factors of 13 further levels (for six of them for the first time).

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