Identification of $n=3$, $\Delta n=0$ Transitions of NeI-Like TiXIII in the Beam-Foil Spectrum of Titanium

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Most of the previously unidentified strong lines in the EUV spectrum of foil-excited titanium have been identified as originating from $n=3$, $\Delta n=0$ transitions of Ti^{12+}. Term values of $n=3$ levels are obtained and compared with theoretical data.

Introduction

The EUV spectrum $9\,nm \leq \lambda \leq 52\,nm$ of foil excited titanium has been observed recently [1]. In that experiment, the ion beam energy (15 to 20 MeV) was optimized for the production of Ti^{11+} according to the prescription given by Sayer [2]. Most of the many lines observed could be identified from the available tabulations [3–5] as belonging to the spectra of TiX, XI, XII and XIV with the notable exception of TiXIII, i.e. Ti^{12+}. It is the aim of this paper to identify lines belonging to the TiXIII spectrum.

The spectrum of Ti^{12+} is neonlike. There are 36 excited levels in the $n=3$ shell which is the lowest shell above the closed shell ground state. These levels result from electron configurations $1s^2 2s^2 2p^5 3l$ and $1s^2 2s 2p^6 3l$, with $l=0,1,2$ (s,p,d). The number of close-lying levels and the considerable fine structure splittings give rise to widely spaced line multiplets which tend to overlap with other multiplets of the same ion, not to mention the many other lines of other ionization stages present in the same spectral range. However, a certain interest in the classification of the spectra arises from the quest for VUV lasers employing neonlike ions [6].

The experimental knowledge of the NeI isoelectronic sequence up to ArIX has been summarized and graphically displayed by Buchet-Poulizac and Buchet [7]. For higher nuclear charges the experimental data are sparse. Some lines have been identified in observing a fast ion beam (Fe[8]), a Z-pinch discharge (Kr[9]) or solar flares (Fe[10], with the aid of calculations, e.g. [11]). At present work is being done at Lund to obtain NeI-like spectra of elements Ti−Fe from a laser-produced plasma [12].

Reference Data

The data evaluated and collected by the Buchets [7] refer to $2s^2 2p^5 3l$ levels only. They can be extrapolated beyond ArIX, but the resulting uncertainty for $Z=22$ (Ti) is rather large for some levels. The same $2s^2 2p^5 3l$ levels have been covered by calculations by Crance [13] who also gives lifetimes. Bureeva and Safronova [14] give all $n=3$ levels $(2s^2 2p^5 3l$ and $2s 2p^6 3l)$ as well as diagrams for level compositions. They group the atomic levels by the L and J values (jK coupling), because some of the multiplets of the LS coupling scheme are hardly recognizable. The results of their *ab-initio* $1/Z$ perturbation theory calculation are presented in a way to infer the variation of multiplet splittings along the isoelectronic series.

Another calculation of all $n=3$ levels was provided upon request by B.C. Fawcett [15] who employed an adaption of a computer program package written by R.D. Crowan [16]. This program involves a Hartree-Fock-Relativistic routine with the Blume-Watson formalism for the spin-orbit part. The Slater integrals in this computation are adjusted heuristically to approximate experimental data. The computer output of this code contains eigenvalues and eigenvectors in LS and jj-coupling as well as a list of all electric dipole transitions together with their wavelengths and transition probabilities. The composition of the eigenvectors indicates many impure states, and a classification of the levels according to their major component in the LS scheme (see Table 1) sometimes disagrees with the sequence of levels given by Bureeva and Safronova whose designation of levels has been adopted here. The tran-

Table 1. States, main components, term values and lifetimes as calculated by Fawcett [15] and by Bureeva and Safronova [14] and experimental values. LS notation is adopted. Electronic configurations: A: $2s^2 2p^6$; B: $2s^2 2p^5 3s$; C: $2s^2 2p^5 3p$; D: $2s^2 2p^5 3d$; E: $2s 2p^6 3s$; F: $2s 2p^6 3p$; G: $2s 2p^6 3d$. The ordering of the levels is by term value [15]. Term values in brackets indicate levels which could not be connected to other levels by $n=3$, $\Delta n=0$ transitions observed here

Configu-ration	Desig-nation [14]	Composition [15]	Lifetime (ps) [15]	Term value (cm⁻¹) [15]	[14]	This work	Comment
A	$^1S_0$	100% $^1S_0$	∞	0	0	0	
B	$^3P_2$	99.8% $^3P_2$	∞	3696 499	3696 300	3698 080	
	$^3P_1$	52.6% $^3P_1$; 47.2% $^1P_1$	2.6	3706 820	3708 220	3709 150	3709 200 [18]
	$^3P_0$	100% $^3P_0$	∞	3743 396	3743 891	3745 200	
	$^1P_1$	52.6% $^1P_1$; 47.2% $^3P_1$	2.2	3751 103	3753 200	3753 600	3753 600 [18]
C	$^3S_1$	90% $^3S_1$; 10% $^3P_1$	354	3882 822	3878 400	3879 370	
	$^3D_2$	62.6% $^3D_2$; 27.4% $^1D_2$, 9.8% $^3P_2$	265	3905 532	3906 681	3906 140	
	$^3D_3$	100% $^3D_3$	234	3908 299	3907 800	3908 820	
	$^3D_1$	43.8% $^1P_1$; 32.7% $^3D_1$, 21.8% $^3P_1$	246	3916 567	3917 285	3918 050	
	$^1D_2$	67% $^3P_2$; 32.7% $^1D_2$	206	3924 306	3925 900	3926 850	
	$^3P_0$	97.6% $^3P_0$; 2.4% $^1S_0$	190	3947 665	3950 425	3949 860	
	$^1P_1$	63.3% $^3D_1$; 33.8% $^1P_1$; 2.6% $^3P_1$	270	3950 599	3952 900	3951 160	
	$^3P_1$	65.1% $^3P_1$; 21.7% $^1P_1$; 9.4% $^3S_1$	214	3962 914	3966 348	3964 850	
	$^3P_2$	39.8% $^1D_2$; 37% $^3D_2$; 23.1% $^3P_2$	227	3963 791	3965 900	3965 450	
	$^1S_0$	97.6% $^1S_0$; 2.4% $^3P_0$	59	4063 658	4062 100	4063 200	
D	$^3P_0$	99.6% $D\,^3P_0$; 0.3% $F\,^3P_0$	108	4164 791	4159 400	4163 800	
	$^3P_1$	94.1% $^3P_1$; 5.3% $^3D_1$	24	4169 203	4163 532	4168 240	4168 240 [18]
	$^3P_2$	79.3% $^3P_2$; 13.3% $^3D_2$; 7% $^1D_2$	111	4177 641	4172 080	4177 080	
	$^3F_4$	100% $^3F_4$	112	4179 852	4174 100	4179 420	
	$^3F_3$	69.5% $^3F_3$; 25% $^1F_3$; 5.5% $^3D_3$	104	4184 485	4177 517	4184 430	
	$^3F_2$	43.7% $^3F_2$; 34.4% $^1D_2$; 21.8% $^3D_2$	101	4192 978	4189 674	4193 940	
	$^1F_3$	60.4% $^3D_3$; 37.4% $^1F_3$; 2.2% $^3F_3$	105	4198 532	4195 200	4199 650	
	$^3D_1$	84.6% $^3D_1$; 11.3% $^1P_1$; 3.9% $^3P_1$	0.7	4219 241	4218 300	(4219 800)	4219 800 [18]
	$^1D_2$	56% $^3F_2$; 29.6% $^1D_2$; 14.2% $^3D_2$	101	4232 234	4229 900	4233 000	
	$^3D_2$	51.6% $^3D_2$; 28.9% $^1D_2$; 20.1% $^3P_2$	105	4236 237	4234 348	4237 450	
	$^3D_3$	37.6% $^1F_3$; 34.1% $^3D_3$; 28.2% $^3F_3$	107	4238 191	4237 879	4238 840	
	$^1P_1$	87.8% $^1P_1$; 10% $^3D_1$; 1.6% $^3P_1$	0.1	4284 325	4286 700	(4281 600)	4281 600 [18]
E	$^3S_1$	99% $E\,^3S_1$; 1% $C\,^3S_1$	2,856	4548 018	4501 400	4530 260	
	$^1S_0$	100% $E\,^1S_0$	670	4586 677	4536 100	(4569 000)	
F	$^3P_0$	99.5% $F\,^3P_0$; 0.3% $D\,^3P_0$	239	4751 542	4730 600	4731 780	
	$^3P_1$	93.9% $^3P_1$; 5.6% $^1P_1$	10.7	4753 547	4732 056	4733 300	4733 300 [19]
	$^3P_2$	99.5% $^3P_2$	211	4760 696	4739 031	4741 030	
	$^1P_1$	93.9% $^1P_1$; 5.6% $^3P_1$	0.6	4772 014	4751 600	4754 000	4754 000 [19]
G	$^3D_1$	100% $^3D_1$	98	5024 794	5021 300	5003 600	
	$^3D_2$	100% $^3D_2$	100	5025 348	5021 736	5004 030	
	$^3D_3$	100% $^3D_3$	104	5026 227	5022 442	5004 740	
	$^1D_2$	100% $^1D_2$	92	5051 419	4930 800	5009 000	

sition probabilities given by Fawcett have been used to estimate line intensities (see below) and to calculate lifetimes of $n=3$ levels (see Table 1). The lifetimes agree satisfactorily with those given by Crance [13].

Few experimental term values are known for Ti XIII. The compilation by Sugar and Corliss [17] relies on two references for the $n=3$ term values: Edlén and Tyrén [18] have set the corner stones by their determination of the $2s^2 2p^5 3s\,^{1,3}P_1$ and $2s^2 2p^5 3d\,^1P_1$, $^3P_1$ and $^3D_1$ term values. Feldman and Cohen [19] have added information by measur-

ing the wavelengths of the ground state transitions from the $2s\,2p^6 3p\,^{1,3}P_1$ levels.

Extension of Experimental Data

There are 224 allowed electric dipole transitions in the $n=2$ groundstate plus $n=3$ level complex. The well known spectral lines corresponding to the seven ground state transitions have wavelengths near 2 nm and are outside the range accessible to the experimental set-up used [1]. The other lines are spread

over a range from about 12 to 70 nm. Our experimental data [1] which have been recorded with appropriate spectral resolution up to $\lambda=53$ nm were extended up to 58 nm to cover the full range of the thirty-odd strongest lines.

The new lines found in this extended spectrum are given in Table 2 as well as new identifications of lines in the range covered previously.

The typical uncertainty of the line positions in the experimental data is of order 0.01 nm (0.005 nm for lines of medium or higher intensity). This corresponds to an uncertainty of term differences of 120 cm^{-1} for lines near 28 nm and of 60 cm^{-1} for lines near 56 nm. For blended lines these uncertainties have to be increased; the maximum uncertainty there is of the order of the spectral resolution (FWHM 0.04 nm). The typical uncertainty of term resolution (FWHM 0.04 nm). The typical uncertainty of term values derived from the analysis given here is about 100 cm^{-1} where at least one well-known level is involved in a decay chain. Otherwise a simultaneous shift of several levels of a decay chain (several levels connected by sufficiently strong transitions but without connections) is possible yielding an error of up to 200 cm^{-1}. This, of course, does not cover the problem of misidentifications.

Preliminary decay curve data have been recorded for four lines which have been assigned to $2s^2 2p^5 3p$ $-2s^2 2p^5 3d$ transitions ($\lambda=33.59$ nm; 35.47 nm; 35.92 nm; 36.57 nm) (see below); the resulting mean lives ($\tau \simeq 115 \pm 20$ ps ($^3P_2$); 130 ± 20 ps ($^1D_2$); 130 ± 20 ps ($^3F_3$); 160 ± 20 ps ($^3D_3$), however, are not particularly significant, as almost all $2s^2 2p^5 3p$ states have mean lives of order 200 ps, and almost all $2s^2 2p^5 3d$ states have mean lives of order 100 ps. A clear discrimination by the lifetime of states in the same subshell therefore is not possible. If the identifications are correct, the experimental mean lives are closer to Fawcett's values ([15], included in Table 1) than to Crance's data [13].

Data Analysis

The available theoretical $n=3$ level schemes [4, 13–15], though similar to each other and to extrapolated experimental data, need to be adjusted to match the experimental term values [17]. In order to facilitate comparisons of theoretically predicted level schemes and experimental spectra, spectra based on theoretical data were simulated. Whereas it is trivial to obtain wavelengths from a level scheme, the prediction of line intensities needs more information. As a first guess, the initial population of the $n=3$ levels has been assumed to be proportional to the statis-

tical weight factor $(2J+1)$ of the individual level irrespective of the excitation energy. Corrections to this simple model which were advisable in the light of the subsequent line identifications turned out to be small: The high-lying $2s 2p^6 3d$ levels appear to be less populated by a factor of three, the population of the $2s^2 2p^5 3d$ levels ought to be reduced by about 10% whilst the lines originating from the lower lying $2s^2 2p^5 3p$ levels indicate a slightly higher initial population or repopulation by cascades.

The theoretical branching ratios for lines corresponding to various transitions from the same upper level were incorporated into the simulation of spectra. In addition the lifetimes of the levels are needed because of the inherent temporal resolution of the fast beam light source. An observed flight path corresponding to 80 ps has been assumed in the simulation to approximate the conditions of the experiment [1]. The detection efficiency curve of the spectrometer plus detector [20] was taken into account.

A visual comparison showed a general similarity of the pattern of previously unidentified lines with the simulated Ti XIII spectrum. However, looking at details, not a single theoretical line position was immediately acceptable as being close enough to experiment. In a tedious trial and error procedure the theoretical term schemes were varied with the aim to match the simulated lines with lines in the observed spectrum. A limitation of this procedure lies in the complexity of the transition arrays and the frequent accidental blendings with other lines of the same or other ionization stages of titanium (within the experimental line width (FWHM) of about 0.04 nm). An advantage of the beam-foil light source is the certainty that all lines belong to ions of one element only.

As a first step in the adjustment of the theoretical level scheme the odd parity levels with total angular momentum equal to unity (i.e. those levels which directly connect to the ground level) have been shifted to match the experimental term values [17]. This means a small shift for $2s^2 2p^5 3s$, $3d$ levels but a major one for $2s 2p^6 3p$ levels [15]. The ground state decay branch of these levels renders the remaining in-shell decays very weak. Therefore the $n=3$, $\Delta n=0$ spectra cannot be tied to all of the well-known levels directly. Nontheless, shifts of levels in the same subshell can be estimated.

Whereas in the different calculations the relative positions of $2s^2 2p^5 3l$ levels are in fair agreement, the situation is much less clear for $2s 2p^6 3l$ levels which are covered in two calculations [14, 15] only. The fact that both calculations include only electronic states up to $n=3$ although the lowest $n=4$ level [4]

Table 2. Lines identified in this work and newly found lines in the extension of the spectrum to higher wavelengths than covered previously [1]. Wavelengths for Ti XIII are those matching the level scheme of Table 1; they may slightly differ from the experimental wavelength values given in [1]. In the column "Transition" the electron configurations of Ti XIII levels have been abbreviated as defined in the legend of Table 1. The line intensities of Ti XIII lines are in arbitrary units close to experimental values with the effect of the detection efficiency variation accounted for [20]. Intensities of other lines are indicated by m (medium), w (weak), or vw (very weak). Where identifications given in this table differ from those given in [1], the present identification is expected to indicate the stronger contribution, because lower-lying excited levels are involved

pb partial blend with line of ...; b blend with line of ...

Wavelength (nm)	Spectrum of Ti	Transition	Line intensity Simulation	Line intensity Experiment	Comment
12.41	XII	$4p-7d$		vw	
14.16	XII	$4d-7f$		vw	
14.57 / 14.66	XII	$4p-6d$		vw	
16.98	XII	$4d-6f$		w	
20.51 − 20.68	XIV	$4-5$		m	
20.71 / 20.85	XII	$4p-5d$		w	
23.72–23.95	XIII	$4-5$		m	
25.29 / 25.31	XII	$4d-5f$		mw	
28.245	XIII	$B\,^3P_1 - C\,^1S_0$	9	9	b Ti VIII
32.300	XIII	$B\,^1P_1 - C\,^1S_0$	13	~15	b Ti VIII, Ti IX
32.196	XIII	$C\,^1D_2 - D\,^3D_2$	4		b
33.590	XIII	$C\,^3S_1 - D\,^3P_2$	31	32	
34.384	XIII	$C\,^3D_3 - D\,^1F_3$	18	23	
34.618	XIII	$C\,^3S_1 - D\,^3P_1$	12	18	
34.746	XIII	$C\,^3D_2 - D\,^3F_2$	23	32	pb Ti XII in 3rd diff. order
35.158	XIII	$C\,^3S_1 - D\,^3P_0$	11	18	pb Ti XII $3p\,^2P_{3/2} - 3d\,^2D_{3/2}$
35.478	XIII	$C\,^1P_1 - D\,^1D_2$	56	56	b Ti XI
35.934	XIII	$C\,^3D_2 - D\,^3F_3$	76	109	
36.20				49	pb higher order of unidentified line
36.246	XIII	$C\,^3D_1 - D\,^3F_2$	40		
36.286	XIII	$C\,^3D_3 - D\,^3F_3$	13		
36.574	XIII	$C\,^3P_2 - D\,^3D_3$	86	91	
36.657	XIII	$C\,^1D_2 - D\,^1F_3$	70	70	
36.684	XIII	$C\,^3P_1 - D\,^3D_2$	50	40	
36.761	XIII	$C\,^3P_2 - D\,^3D_2$	6	7	
36.789	XIII	$F\,^3P_0 - G\,^3D_1$	7		b
36.909	XIII	$C\,^3D_2 - D\,^3P_2$	3		
36.937	XIII	$F\,^3P_1 - G\,^3D_2$	19	144	
36.955	XIII	$C\,^3D_3 - D\,^3F_4$	110		
36.996	XIII	$F\,^3P_1 - G\,^3D_1$	5		
37.369	XIII	$C\,^3P_2 - D\,^1D_2$	6	12	b Ti?
37.485	XIII	$B\,^3P_2 - C\,^3P_1$	3	12	b Ti?
37.920	XIII	$F\,^3P_2 - G\,^3D_3$	34	56	b
37.908	XIV	$5-6$			
−38.016				35	
38.023	XIII	$F\,^3P_2 - G\,^3D_2$	6		
38.606	XIII	$C\,^3D_1 - D\,^3P_2$	4	110	b Ti XI
39.216	XIII	$F\,^1P_1 - G\,^1D_2$	26	39	tentative
39.963	XIII	$C\,^1D_2 - D\,^3P_2$	20	23	pb Ti IX
41.544	XIII	$B\,^3P_1 - C\,^3P_0$	8	28	b Ti XI
43.712	XIII	$B\,^3P_2 - C\,^1D_2$	28	48	
44.06–44.14	XIII	$5-6$			
45.527	XIII	$B\,^3P_0 - C\,^3P_1$	14	16	
45.935	XIII	$B\,^3P_1 - C\,^1D_2$	20	24	pb Ti IX
47.209	XIII	$B\,^1P_1 - C\,^3P_2$	42	36	
47.337	XIII	$B\,^1P_1 - C\,^3P_1$	11	14	b 2nd order
47.445	XIII	$E\,^3S_1 - F\,^3P_2$	43	106	
47.452	XIII	$B\,^3P_2 - C\,^3D_3$	60		
47.870	XIII	$B\,^3P_2 - C\,^3D_1$	22	23	
48.063	XIII	$B\,^3P_1 - C\,^3D_2$	19	33	b Ti VIII
48.553	XIII	$B\,^3P_0 - C\,^1P_1$	11	11	

Table 2 (continued)

Wavelength (nm)	Spectrum of Ti	Transition	Line intensity		Comment
			Simulation	Experiment	
49.251	XIII	$E\,^3S_1 - F\,^3P_1$	3	6	
49.623	XIII	$E\,^3S_1 - F\,^3P_0$	8	15	
50.618	XIII	$B\,^1P_1 - C\,^1P_1$	12	10	
50.764	XIII	$B\,^3P_1 - C\,^3D_2$	20	28	
51.722	XII	$5g - 6h$		mw	
51.82				vw	
52.04				w	
52.27				w	
52.48				vw	
52.65/53.71				vw	
52.89				vw	
53.02				vw	
53.345				w	
53.74				vw	
54.01				vw	
54.36				vw	
54.905				vw	
55.160	XIII	$B\,^3P_2 - C\,^3S_1$	16	14	
55.816	XII	$4f - 5g$			2nd order
57.65				vw	

is rather close to the $2s\,2p^6\,3d$ levels, may account for part of the deviation:

Fawcett's data show the normal singlet-triplet separation and $3s-3p-3d$ term differences of the $2s\,2p^6\,3d$ levels, although the calculated levels appear to lie too high. The data of Bureeva and Safronova, however, are probably in error for these levels. Their $3s-3p$ term differences are much larger than those of the $2s^2\,2p^5\,3s$, $3p$ levels, and the $2s\,2p^6\,3d\,^1D_2$ level is given with a term value much below the $^3D_{1,2,3}$ levels, contrary to expectation from the structure of the lower subshells. The line identifications proposed in this work are close to Fawcett's term structure except for the shift mentioned.

Most of the 217 lines which correspond to $n=3$, $\Delta n=0$ transitions are weaker than 1 % of the strongest line (according to the above prescription) $2s^2\,2p^5\,3p\,^3D_3 - 2s^2\,2p^5\,3d\,^3F_4$. These weak lines hardly exceed the background level and have been neglected in the present analysis. The thirty-odd strongest lines (except g.s. transitions) all lie in the wavelength interval $28\,\mathrm{nm} \leqq \lambda \leqq 60\,\mathrm{nm}$ where indeed most of the medium intensity or even strong lines which could not be identified previously are to be found.

Where several line identifications were possible, the level assignment approximating the multiplet splittings of Bureeva and Safronova [14] has been adopted. The resulting term values are listed in Table 1. The line identifications are given in Table 2.
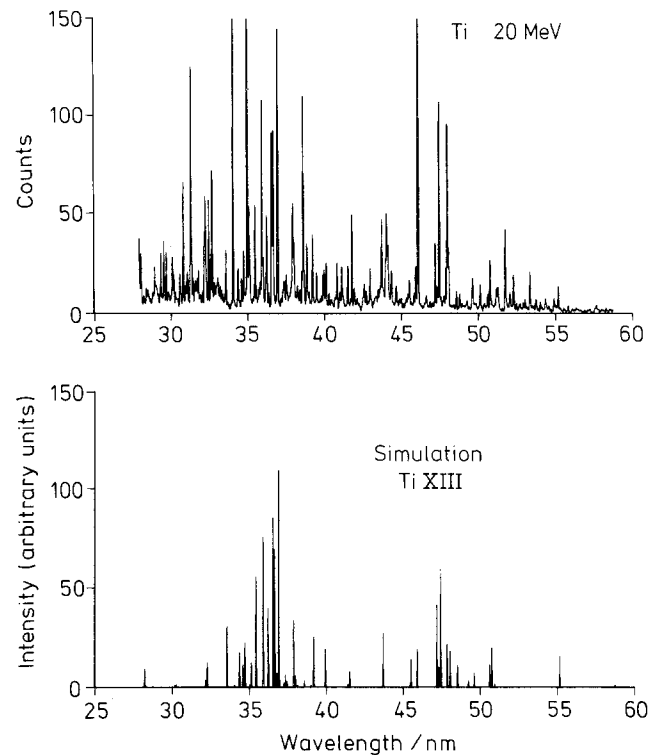

Fig. 1. a Spectrum of foil-excited titanium in the wavelength range 27–58 nm. The spectrum contains lines of Ti VIII–XIV. **b** Simulated spectrum of Ti XIII according to the adopted term scheme. Blended lines are drawn individually. They are not added to give resultant intensities
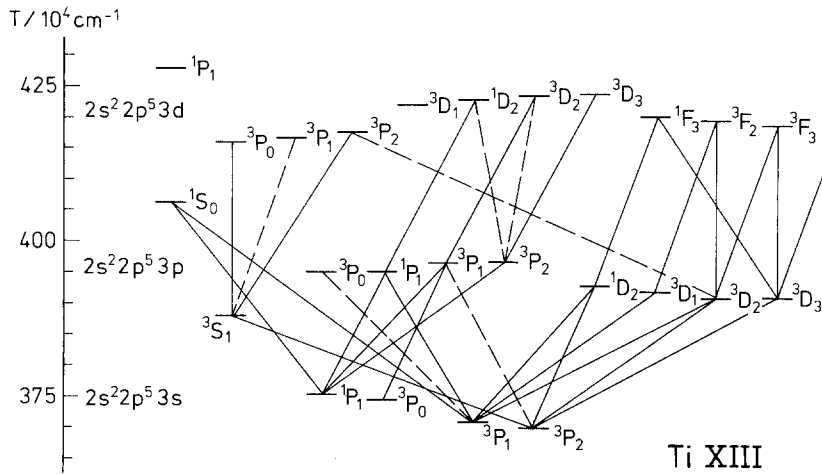
Fig. 2. Level scheme of Ti XIII $2s^2 2p^5 3l$ levels. Solid lines represent $n=3$, $\Delta n=0$ transitions which are strong enough to contribute a detectable line to the spectrum. Broken lines represent rather weak transitions. Term values of levels without interconnections within the $n=3$ shell are known from the ground state transitions [17, 18]

Because of a certain degree of arbitrariness in several identifications a few comments will be given:

The experimental spectrum in the range 28–58 nm (Fig. 1) contains many known lines from charge states other than Ti^{12+}. These lines serve as calibration lines in the wavelength determination of the new lines. Relative line intensities in the multiplets of known spectra closely agree with the well-known rules [21]. The linewidth is predominantly determined by the instrumental resolution with a small Doppler broadening contribution. Hence it is fairly straightforward to detect significant blends with unknown lines by apparent shifts of wavelengths of known lines (in n^{th} diffraction order), an increased line with, or a deviation from the usual line intensity pattern.

It turns out that only few of the significant lines of Ti XIII are blended with lines of other spectra, but there are several blends within the Ti XIII spectrum. If a level connects to other levels via several transitions, the blend of a single of these transitions with a foreign one may be inferred. However, Fig. 2 shows the pattern of connecting transitions in the $2s^2 2p^5 3l$ arrays giving rise to lines which are strong enough to be detectable in our spectra. It is obvious from this pattern that the $2s^2 2p^5 3d\,^1P_1$, $^3D_1$ levels cannot be crossreferenced with any of the other levels of the array, because they decay to the ground state almost exclusively. The $2s^2 2p^5 3d\,^3P_1$ level with its weaker g.s. transition decay branch may still be seen via its decay by $n=3$, $\Delta n=0$ transition to $2s^2 2p^5 3p\,^3S_1$.

Several $3d$ levels connect to only one $3p$ level which in turn may connect to only one of the $3s$ levels. There are only very few closed loops of transitions which permit to cross-check certain line identifications. The $2s^2 2p^5 3p\,^1S_0$ level, for example, can decay to the known reference levels $2s^2 2p^5 3s\,^1P_1$ and $^3P_1$.

The energy difference of the two transitions therefore is known to be equal to the term difference of the $3s^{1,3}P_1$ levels. A search in the wavelength range suggested by the calculations shows identification problems because the two spectral lines are expected to be rather weak. Despite of the high density of weak lines in this range of the spectrum there are few lines with the proper difference in energy. An identification is suggested here based on a proper intensity match of simulation and experiment for the short wavelength line and a partial blend of the longer wavelength line with a line of Ti VIII. The resulting $3p\,^1S_0$ term value is close to Fawcett's prediction (the same holds for all term values given for the $2s^2 2p^5 3p$ levels except for $^3S_1$). An alternative suggestion for the wavelengths of the two lines originating from $3p\,^1S_0$ has been given by Kastner [22]. Those wavelengths, based on a semiempirical extrapolation, are higher by about 0.4 nm, but in the range of Kastner's estimated uncertainty (about 0.1–0.13 nm) around his expected value no matching line pair could be found. One of the less suited alternatives would lower the $3p\,^3S_1$ level by 2800 cm^{-1} compared to the value given in Table 1.

There is a particular interest in the term value of this level and of the $2s^2 2p^5 3p\,^3P_0$ level as transitions from those levels $(3s\,^1P_1 - 3p\,^1S_0$, $3s\,^3P_1 - 3p\,^3P_0)$ have been considered to provide likely candidates for UV laser lines [23]. The low intensities of both lines are a disadvantage in the quest of their identification. Any higher resolution work will be very time-consuming.

At 47.45 nm a rather strong line appears in the spectrum which cannot be accounted for by any single transition. The intensity of this line, however, nicely matches the sum of the intensities of at least two lines of Ti XIII which can be assumed to contribute to this blending.

The term values of the $2s\,2p^6\,3l$ levels relate to the $2s\,2p^6\,3p\,^1P_1$, $^3P_1$ levels determined by Feldman and Cohen [18]. The fast g.s. decay of $^1P_1$ suppresses the transition to $2s\,2p^6\,3s\,^1S_0$. That level cannot be determined in the present work, the term value given in Table 1 implies a shift of Fawcett's calculated term value [15] by as much as the $^3S_1$ level needs to be shifted and should not be interpreted as being more than a rough estimate. Decays from $2s\,2p^6\,3s$ levels are, in principle, observable near $\lambda \simeq 12$ nm as are other $2s^2\,2p^5\,3l - 2s\,2p^6\,3l$ transitions. The predicted intensities, however, are rather low, and the lines are, at least partly, blended by much stronger lines in this wavelength range.

Transitions between $2s\,2p^6\,3l$ levels have rarely been observed in the Ne I sequence. Jupén [24] identified 6 such transitions in Cl VIII which were close to the wavelengths predicted by Bureeva and Safronova [14]. The identification of the $3p\,^1P_1 - 3d\,^1D_2$ transition supports the calculation as to the relative position of the $3d\,^1D$ level being lower than the $3d\,^3D$ levels in Cl VIII. Along the isoelectronic sequence the $3d\,^1D$ level drops considerably (on a relative scale), and for Ti XIII the predicted wavelength of the $3p\,^1P_1 - 3d\,^1D_2$ transition would be 55.8 nm according to [14] (compared to 35.8 nm [15]). No likely candidate line has been found anywhere near this region, with the exception of possible blends with other strong lines (eg. Ti XII $3s - 3p_{1/2,3/2}$ at 46.7 nm and 47.99 nm or the line 47.45 nm which is assumed to be a blend of at least two other lines). If on the other hand Fawcett's calculation [15] with the $3d\,^1D$ level above $3d\,^3D$ comes closer to truth for Ti XIII, the wanted line would be expected in the range 35–40 nm, with a number of single unidentified lines to choose from. The term value given in Table 1 is based on intensity estimates and the assumption that for this particular level multiplet the Fawcett data [15] might be preferable.

For the transitions among $2s\,2p^6\,3l$ triplet levels one expects two groups of lines as observed for the $2s^2\,2p^5\,3l$ levels, the $3s - 3p$ transitions lying near 48–50 nm and the $3p - 3d$ transitions lying in the range 35–40 nm. The 47.45 nm line is so intense that in comparison with other lines of the same multiplet the $2s^2\,2p^5\,3s\,^3P_2 - 2s^2\,2p^5\,3p\,^3D_3$ transition cannot be its only origin. However, there are two weak lines at 49.25 nm and at 49.62 nm which together with the "surplus" intensity of the 47.45 nm line show the intensity pattern expected for the $2s\,2p^6\,3s\,^3S_1 - 2s\,2p^6\,3p\,^3P^0_{0,1,2}$ multiplet and which imply $3p\,^3P^0$ fine structure intervals close to both available calculations [14,15]. The overall intensity of these lines is higher than expected by about a factor of 1.5.

If this multiplet is correctly identified, one can search for the $3p\,^3P^0 - 3d\,^3D$ multiplet. The line splitting of this multiplet is dominated by the $3p\,^3P^0$ fine structure obtained from the $3s\,^3S - 3p\,^3P^0$ multiplet. It is not easy to accommodate the $3p - 3d$ multiplet in the envelope of the measured spectrum because 5 of its 6 components exceed the typical background level even at the assumed relatively low population of the $3d$ levels. The identification chosen here localizes the weak $^3P^0_0 - ^3D_1$ line near 36.57 nm, the $^3P^0_1 - ^3D_{1,2}$ components blended with a very strong line at 36.96 nm (and hence not visible) and the strongest $^3P^0 - ^3D_3$ component near 37.92 nm blended with another line multiplet. That multiplet is tentatively ascribed to Ti XIV 5–6 yrast transitions based on a wavelength estimate; it appears somewhat stronger than expected from the charge state distribution [2] in comparison with the 5–6 yrast transitions of Ti XIII (near 44 nm) and Ti XII (51.7 nm) and thus would agree with the assumption of a blend.

Comparison with Theory

There are some general deviations among the available calculated level schemes and the experimental level scheme derived in this work. (A graphical representation of the data would take up too much space here.)

For the $2s^2\,2p^5\,3s$ levels, the calculations by Crance [13] yield a $^3P_0 - ^1P_1$ interval which is too small and a $^3P_2 - ^3P_1$ interval which is far too large. The experimental splittings are somewhat intermediate to Fawcett's [15] data and those by Bureeva and Safronova [14]. For the $2s^2\,2p^5\,3p$ levels the data by Crance show a slightly too large spacing of all levels – whereas the P levels are about right, the D levels are considerably too low and the $^1S_0$ level is much too high. In Fawcett's data only the $^3S_1$ level is significantly too high. The most significant deviation of the Bureeva and Safranova prediction from the result of this analysis is the sequence of highest P levels: they give $^3P_1$ higher than $^3P_2$ (with the changeover of the two levels occurring near $Z=23$ in the isoelectronic sequence), whereas the experiment agrees with the other calculations ($^3P_2$ higher than $^3P_1$).

For the $2s^2\,2p^5\,3d$ levels the term structure given by Crance grossly deviates from the others and from experiment. Here the calculation by Bureeva and Safronova distinctly shows an excessive mean term separation (about 8%). If one corrects for that, the actual structure is again intermediate between their data and those by Fawcett.

For the $2s\,2p^6\,3l$ levels the suspected shortcomings

of the Bureeva and Safronova data on the even parity levels have already been mentioned. However, their data are fairly good for the odd parity levels. After introducing a shift to Fawcett's term values for these levels, they give the best overall agreement.

In conclusion, the present level scheme derived from line identifications confirms theoretical predictions [14, 15] with some significant exceptions for a few levels. Modified average level spacings in specific subshells permit to use the theoretical data with greater predictive power for higher Z elements.

In parallel to the present analysis Jupén and Litzén [12] have performed extensive experimental and computational isoelectronic studies of the NeI sequence [25, 26] which were finished almost coincidently with the main part of the present analysis. Their laser -produced plasma data for a series of elements remove ambiguities in several key line identifications which are crucial for this study. Some preliminary identifications of transitions between $2s^2 2p^5 3l$ levels have been corrected and now all agree with the results obtained by Jupén and Litzén [25].

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