IOP PUBLISHING PHYSICA SCRIPTA

Phys. Scr. **80** (2009) 065302 (4pp) doi:10.1088/0031-8949/80/06/065302

Extension of the resonance line series of Mg III

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Received 9 June 2009
Accepted for publication 16 October 2009
Published 1 December 2009
Online at stacks.iop.org/PhysScr/80/065302

Abstract
Spectra of Mg emitted by a Penning discharge were recorded in the extreme ultraviolet (EUV) on a 10.7-m grazing-incidence spectrograph with phosphor image plates. The spectra provided nine new lines of Mg III between 156 and 166 Å and allowed us to improve previous wavelength measurements for another seven lines in this spectral region.

PACS numbers: 32.10.Fn, 32.30.Jc, 32.80.Ee, 95.30.Ky

1. Introduction

Mg^{2+} is a member of the neon isoelectronic sequence. Its ground state is $2s^22p^6\,{}^1S_0$, so the resonance transitions are of the type $2s^22p^6$–$2s^22p^5\,ns$, nd. The spectrum of Mg^{2+} was previously compiled by Kaufman and Martin [1]. The energy levels used in this compilation were compiled earlier by Martin and Zalubas [2]. Those compilations were mainly based on the analysis of the Mg III spectrum by Andersson and Johannesson [3] and the measurements of the resonance line series in the extreme ultraviolet (EUV) region by Lundström [4]. Since then, no new experimental investigations of the $2s^22p^5nl$ levels of Mg^{2+} were published.

The present work was undertaken with a primary goal of wavelength calibration of the EUV imaging spectrometer (EIS) [5]. For this purpose, improved wavelength measurements and identifications of spectral lines of singly and multiply ionized magnesium and neon were required. Therefore, we investigated the spectrum of a Ne/Mg Penning discharge with the 10.7 m grazing-incidence spectrograph at the National Institute of Standards and Technology (NIST).

2. Experimental

Most of the experimental details were already given in our previous paper [6] on the Ne II spectrum. For the present work, in addition to the Penning discharge lamp described in [6], we took additional spectra with another Penning discharge lamp constructed identically to the one described by Heise *et al* [7]. This lamp had electrodes made of the same Mg/Al alloy (97% Mg and 3% Al) as in [6]. Compared to the lamp used in [6], this new lamp was operated at much higher electric currents, which resulted in greater erosion of the magnesium electrodes. As a result, the relative intensity of magnesium spectral lines was greatly enhanced compared to our previous spectra. This allowed us, just by comparison of relative line intensities, to distinguish magnesium lines from neon ones with 95% certainty.

The spectra were recorded on Fuji phosphor storage image plates type BAS-TR2040[4] and converted to digital images using a Perkin Elmer Cyclone reader model B431200 laser scanner. The digital images, having a resolution of 600 dpi, were integrated over the height of spectral lines and converted to plots of intensity versus pixel number corresponding to the length coordinate in the direction of spectral dispersion. An automatic measuring program [8] was used to fit spectral line shapes to Gaussian or Voigt profiles. The program output was a list of fitted centroids, widths and areas of the lines. The overall sensitivity of the registration was almost flat in the studied wavelength range 156–166 Å. The pixel size in the recorded image is $\approx 40\,\mu$m (corresponding to ≈ 0.01 Å), and sharp, unblended lines had a full-width-at-half-maximum (FWHM) of 2.5 pixels (0.017–0.025 Å). The fitted line centroids were reproducible to better than 0.1 pixels (0.001 Å).

[4] Commercial products are identified in this paper for adequate specification of the experimental procedure. This identification does not imply recommendation or endorsement by NIST or NRL, nor that they are necessarily the best available for the purpose.

Well-measured Ne II–IV [9–11] and Mg IV [12] lines together with lines from Y [13] and Mo [14–16] ions, which were superimposed on some of the spectra using a sliding spark discharge, were used for wavelength calibration. The standard wavelengths were fitted by least squares to polynomials. Normally, polynomials of order 8–10 were required to remove systematic shifts caused by deformation of the image plates. Spectra from up to six plates were averaged for many spectral lines. Several lines were also measured in the second order of diffraction on one or two plates. The second-order measurements of the lines with high signal-to-noise ratio (S/N) were given twice the weight in the wavelength averaging. Outlying measurements were eliminated from the averages. The total wavelength-measurement uncertainty was determined as a combination of the statistical and systematic uncertainties. The systematic uncertainty, determined by the accuracy of the reference lines and deviations of the fitted wavelengths from the reference values, is estimated to be ±0.002 Å. Statistical uncertainty of unblended lines is inversely proportional to S/N. It was negligibly small for the strongest lines but could reach up to 0.015 Å for the weakest lines with S/N ≈ 1. Intensities of the lines measured on several exposures with different Penning lamps and different discharge conditions were normalized to a common scale. This scale corresponds to the exposure at which relative intensities of magnesium lines were the greatest.

3. Calculations

In order to predict the expected positions and approximate relative intensities of previously unobserved lines of Mg^{2+}, we made a parametric fitting of the known energy levels of this ion using Cowan's atomic structure codes [17] without relativistic corrections. The experimental level values were taken from the compilation of Martin and Zalubas [2]. In this fitting we included the following odd-parity configurations: $2s^22p^5nl$ ($n = 3$–11, $l = 0, 2, 4$) and $2s2p^6np$ ($n = 3$–11). The spin–orbit parameters ζ_{2p} of all configurations were linked together, so that their ratios for different configurations remained fixed at the Hartree–Fock values. A similar grouping was made for the $G^1(3p, ns)$ parameters of the $2p^5\,ns$ configurations and for $F^2(2p, nd)$, $G^1(2p, nd)$, and $G^3(2p, nd)$ of the $2p^5\,nd$ configurations. As a result of the fitting, 60 known odd-parity levels of the $2p^5nl$ configurations were fitted with 17 free parameters and with standard deviation of the calculated levels from experimental ones amounting to 21 cm^{-1}. Then we extrapolated the resulting ratios (fit/HF) of the average energies of the known $2p^5nl$ configurations to find approximate scaling factors for unknown highly excited configurations. This allowed us to predict the positions of unknown levels with uncertainties of about 50 cm^{-1}. This corresponds to the uncertainty of about 0.015 Å in predicted wavelengths of the $2p^6$–$2p^5nl$ transitions and was sufficient to identify the unknown lines in our spectra. Besides that, the fitting provided us with percentage compositions of the eigenvectors in the LS and J_1K coupling schemes and with approximate values of transition rates.

These calculations allowed us to identify the weak, previously unobserved, lines corresponding to transitions $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{3/2})nd\,{}^2[3/2]^\circ_1$ ($n = 10, 11$), $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{3/2})nd\,{}^2[3/2]^\circ_1$ ($n = 6$–8), $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{1/2})ns\,{}^2[1/2]^\circ_1$ ($n = 7, 8$) and $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{3/2})ns\,{}^2[1/2]^\circ_1$ ($n = 7$–9).

In order to verify the identifications, we made a Rydberg analysis of the series by fitting the Ritz-type quantum-defect expansion formulae. For these calculations, we used the computer code RITZPL by Sansonetti [18]. The formula that we used is as follows:

$$\delta_n = c_0 + c_1/(n-\delta_n)^2 + c_2/(n-\delta_n)^4 + \cdots, \qquad (1)$$

where δ_n is the quantum defect defined by the following expression:

$$E_{\rm lim} - E_n = RZ_c^2/(n-\delta_n)^2, \qquad (2)$$

where $E_{\rm lim}$ is the series limit, R is the Rydberg constant. Z_c is the effective charge of the ionic core (for Mg III, $Z_c = 3$), n is the principal quantum number and E_n is the excitation energy.

In our quantum-defect fittings, the ionization limits were fixed to the values 646 402 cm^{-1} for the $2s^22p^5({}^2P^\circ_{3/2})nl$ and 648 631 cm^{-1} for the $2s^22p^5({}^2P^\circ_{1/2})nl$ series [2]. Since the high-n lines are very faint and have large measurement uncertainties, the expansion in formula (1) was restricted to two terms, except for the $2s^22p^5({}^2P^\circ_{3/2})ns\,{}^2[3/2]^\circ_1$, for which we used a three-term formula. All measurements were given equal weights in the fit. The fitting resulted in reasonably small deviations of experimental level values from the fitted ones. The average deviations for different series were between 8 and 26 cm^{-1}. Their smallness and the absence of abnormally large deviations confirmed all new identifications. Since fitting of the quantum-defect expansion with a fixed value of the series limit is in effect an interpolation, the fitted values of the highest levels are probably more accurate than the measured ones. However, there may be occasional perturbations of the series caused by configuration interactions. For example, the $2s^22p^5({}^2P^\circ_{3/2})nd\,{}^2[3/2]^\circ_1$ series is perturbed at $n = 10$ by an interaction with the $2s^22p^5({}^2P^\circ_{1/2})9d\,{}^2[3/2]^\circ_1$ state. For this reason, the $n = 10$ level was excluded from the fitting of the $2s^22p^5({}^2P^\circ_{3/2})nd\,{}^2[3/2]^\circ_1$ series.

4. Results

The measured wavelengths and intensities, as well as the level values derived from them are summarized in table 1. Results of previous measurements by Lundström [4] are included for comparison. Our new measurements agree well with the previous ones. For the lower members of the series, our measured wavelengths are slightly less accurate than the previous ones, mainly because fitting the reference lines with higher-degree polynomials increases the systematic errors. However, because of the great dynamic range of the image plates, we were able to measure the higher members of the series with sufficiently high S/N, thus permitting an improvement over the previous measurements.

Our measured wavelength and energy values of the Mg III resonance lines are given in table 1. They are compared with previous measurements where available. The improved

Table 1. Resonance line series of Mg III in the EUV.

n	λ_{obs}[a] (Å)	I_{obs}	λ_{prev}[b] (Å)	λ_{Ritz}[c] (Å)	E_{exp}[d] (cm^{-1})	E_{calc}[e] (cm^{-1})	1st%[f]	2nd% (J_1K)		1st%		2nd%	(LS)	Note
	$2s^22p^5(^2P^\circ_{1/2})nd\ ^2[3/2]^\circ_1$ series													
3	186.5129(21)	269	186.5149(20)	186.5143(10)	536 152.0(30)	536 155(14)	87	12	$(^2P^\circ_{3/2})3d\ ^2[1/2]^\circ$	62	$^1P^\circ$	36	$^3D^\circ$	
4	170.8044(23)	111	170.8050(20)	170.8041(9)	585 466.2(30)	585 447(14)	92	7	$(^2P^\circ_{3/2})4d\ ^2[1/2]^\circ$	57	$^1P^\circ$	37	$^3D^\circ$	
5	164.3937(23)	38	164.394(2)		608 295(7)	608 310(14)	94			47	$^1P^\circ$	42	$^3D^\circ$	
6	161.1080(23)	17	161.108(2)		620 702(8)	620 703(14)	92	6	$(^2P^\circ_{3/2})7s\ ^2[3/2]^\circ$	42	$^3D^\circ$	41	$^1P^\circ$	
7	**159.2006(21)**	6	159.198(5)		**628 138(8)**	628 156(14)	98			47	$^3D^\circ$	39	$^1P^\circ$	Improved
8	**157.9841(24)**	4	157.981(5)		**632 975(10)**	632 982(14)	98			48	$^3D^\circ$	37	$^1P^\circ$	Improved
	$2s^22p^5(^2P^\circ_{3/2})nd\ ^2[3/2]^\circ_1$ series													
3	187.1965(21)	197	187.1977(20)	187.1966(11)	534 197.7(30)	534 194(15)	79	16	$^2[1/2]^\circ$	62	$^3D^\circ$	37	$^1P^\circ$	
4	171.3931(22)	78	171.3946(20)	171.3941(9)	583 450.5(30)	583 472(15)	74	21	$^2[1/2]^\circ$	58	$^3D^\circ$	41	$^1P^\circ$	
5	164.9472(23)	38	164.949(2)		606 248(7)	606 244(15)	71	26	$^2[1/2]^\circ$	49	$^1P^\circ$	48	$^3D^\circ$	
6	161.6553(23)	27	161.655(2)		618 601(8)	618 579(15)	69	29	$^2[1/2]^\circ$	55	$^1P^\circ$	42	$^3D^\circ$	
7	159.7446(22)	13	159.741(2)		626 013(8)	625 997(15)	67	32	$^2[1/2]^\circ$	58	$^1P^\circ$	39	$^3D^\circ$	
8	**158.5275(23)**	7	158.522(5)		**630 805(9)**	630 802(15)	65	34	$^2[1/2]^\circ$	60	$^1P^\circ$	36	$^3D^\circ$	Improved
9	**157.703(3)**	4	157.701(5)		**634 103(12)**	634 090(15)	60	37	$^2[1/2]^\circ$	60	$^1P^\circ$	33	$^3D^\circ$	Improved
10	**157.118(3)**	4			**636 465(12)**	636 438(15)	48[g]	38	$^2[1/2]^\circ$	54[g]	$^1P^\circ$	27	$^3D^\circ$	New
11	**156.700(10)**	1			**638 160(40)**	638 174(15)	67	31	$^2[1/2]^\circ$	61	$^1P^\circ$	35	$^3D^\circ$	New
	$2s^22p^5(^2P^\circ_{3/2})nd\ ^2[1/2]^\circ_1$ series													
3	188.5311(24)	24	188.5296(20)	188.5296(11)	530 420.6(30)	530 418(26)	72	20	$^2[3/2]^\circ$	97	$^3P^\circ$	2	$^3D^\circ$	
4	171.8991(22)	8	171.8984(20)	171.8997(9)	581 734.7(30)	581 755(26)	72	24	$^2[3/2]^\circ$	93	$^3P^\circ$	5	$^3D^\circ$	
5	**165.191(4)**	2	165.192(5)		**605 359(15)**	605 339(26)	71	28	$^2[3/2]^\circ$	90	$^3P^\circ$	9	$^3D^\circ$	Improved
6	**161.792(8)**	1			**618 076(30)**	618 048(26)	69	30	$^2[3/2]^\circ$	87	$^3P^\circ$	12	$^3D^\circ$	New
7	[159.831(7)][h]	m Ne IV				**625 661**(26)	67	32	$^2[3/2]^\circ$	85	$^3P^\circ$	14	$^3D^\circ$	New
8	**158.593(11)**	2			**630 540(50)**	630 576(26)	65	34	$^2[3/2]^\circ$	83	$^3P^\circ$	15	$^3D^\circ$	New
	$2s^22p^5(^2P^\circ_{1/2})ns\ ^2[1/2]^\circ_1$ series													
3	231.7323(21)	9699	231.7333(20)	231.7336(16)	431 530.0(30)	431 530(8)	56	44	$(^2P^\circ_{3/2})3s\ ^2[3/2]^\circ$	95	$^1P^\circ$	5	$^3P^\circ$	
4	182.2423(20)	346	182.2415(20)	182.2421(10)	548 720.7(30)	548 715(8)	90	10	$(^2P^\circ_{3/2})4s\ ^2[3/2]^\circ$	64	$^1P^\circ$	35	$^3P^\circ$	
5	169.1438(23)	40	169.1406(20)	169.1416(9)	591 220.7(30)	591 231(8)	98			53	$^3P^\circ$	46	$^1P^\circ$	
6	**163.562(3)**	7bl Ne IV	163.562(5)		**611 390(9)**	611 393(8)	99			60	$^3P^\circ$	40	$^1P^\circ$	Improved
7	**160.637(3)**	3			**622 522(16)**	622 527(8)	100			63	$^3P^\circ$	37	$^1P^\circ$	New
8	**158.898(7)**	1			**629 335(30)**	629 321(8)	100			64	$^3P^\circ$	36	$^1P^\circ$	New
	$2s^22p^5(^2P^\circ_{3/2})ns\ ^2[3/2]^\circ_1$ series													
3	234.2618(21)	13326	234.2631(20)	234.2644(16)	426 868.1(30)	426 868(13)	56	44	$(^2P^\circ_{1/2})3s\ ^2[1/2]^\circ$	95	$^3P^\circ$	5	$^1P^\circ$	
4	182.9721(20)	239	182.9717(20)	182.9720(10)	546 531.6(30)	546 534(13)	90	10	$(^2P^\circ_{1/2})4s\ ^2[1/2]^\circ$	64	$^3P^\circ$	35	$^1P^\circ$	
5	169.7441(22)	39	169.7411(20)	169.7427(9)	589 126.8(30)	589 122(13)	98			53	$^1P^\circ$	46	$^3P^\circ$	
6	**164.1318(21)**	7	164.133(5)		**609 267(8)**	609 248(13)	97			59	$^1P^\circ$	39	$^3P^\circ$	Improved
7	**161.2014(22)**	9			**620 342(8)**	620 355(13)	94			59	$^1P^\circ$	35	$^3P^\circ$	New
8	**159.461(5)**	2			**627 113(20)**	627 131(13)	99			64	$^1P^\circ$	35	$^3P^\circ$	New
9	**158.340(15)**	1			**631 552(60)**	631 568(13)	100			65	$^1P^\circ$	35	$^3P^\circ$	New

[a] Present measurements.

[b] From Lundström [4].

[c] From the energy levels optimized by Andersson and Johannesson [3].

[d] Level values from Andersson and Johannesson [3] and Lundström [4], except for the bold-face values, which were determined in the present work.

[e] Level values determined in the present work by fitting a quantum-defect expansion formula with ionization limits fixed to the values 646 402 cm^{-1} ($2p^5\ ^2P^\circ_{3/2}$) and 648 631 cm^{-1} ($2p^5\ ^2P^\circ_{1/2}$) [2] (see text). The values in parentheses are standard deviations of the fitting in the units of the last given decimal figure.

[f] Percentage compositions of the eigenvectors calculated in the present work by parametric fitting using Cowan's codes [17] (see text). Contributions less than 5% are omitted. The first percentage value in the J_1K coupling corresponds to the configuration specified in the series label (the principal quantum number is given in the first column). After the value of the second percentage, the term designation of the second contributing eigenstate is given. If its configuration is different from the series label, it is given before the term. The $2s^22p^5$ core shell designations are omitted for brevity.

[g] The third component is 12% $2p^5(^2P^\circ_{1/2})$ 9d $[3/2]^\circ$ in J_1K coupling or 6% $2p^59d\ ^1P^\circ$ in LS coupling. Due to this perturbation, the 10d $[3/2]^\circ$ level was excluded from the fitting of the quantum defects of the $nd\ [3/2]^\circ$ series.

[h] The wavelength was calculated in this work by fitting a quantum-defect expansion formula (see text).

or new values are given in bold face with a corresponding note in the last column.

In our spectra, the $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{3/2})7d\,{}^2[1/2]^\circ_1$ transition was masked by a moderately intense line of Ne IV at 159.8688(23) Å. For this transition, we included in table 1 the calculated value obtained from the fitting of the quantum-defect expansion formulae (1) and (2). The line at 163.562(3) Å corresponding to the $2p^6\,{}^1S_0$–$2s^22p^5({}^2P^\circ_{1/2})6s\,{}^2[1/2]^\circ_1$ transition was blended in our spectra by a Ne IV line at 163.546(3) Å. We obtained the wavelengths of both these lines by decomposing the blended line profile and averaging the resulting peak positions over five different exposures.

The observed relative intensities of the lines given in table 1 roughly correspond to the S/N ratio and are proportional to the energy flux within the line profile. They do not account for the dependence of the detection sensitivity on wavelength, although this dependence is known to be rather smooth and not very steep [6].

Acknowledgments

We are grateful to G Nave and C Sansonetti for their assistance in conducting this research. The work at NIST was supported in part by the Office of Fusion Energy Sciences of the US Department of Energy and by the National Aeronautics and Space Administration (NASA). The NRL portion of this work was supported in part by the NASA funded part of the EIS Solar B program.

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