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The Auger (autoionization) spectra excited by argon and neon ion bombardment of a magnesium surface

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Abstract. The Auger (autoionization) spectra produced by bombarding a magnesium target with argon and neon ions of energy in the range 200 eV–5 keV are reported. The observed spectra of both gases contained considerable fine structure broadly similar to that observed in spectra from aluminium and silicon targets. The Mg spectra contained structure not previously reported, which could be indexed as part of a series of transitions from an excited state in Mg^0 to states at and above the ground state in Mg^+. The variation of the heights of the main peaks was examined as a function of incident ion energy. The graph of peak height against incidence energy showed a sharp maximum for Ar while this was not the case for either Ne or Mg.

The rare gas Auger peaks increased in energy with increasing incident ion energy and the shift could be explained in terms of a simple Doppler model appropriate to the strongly forward scattered experimental conditions used here. No systematic variation in the energies of the Mg peaks was observed.

1. Introduction

Auger spectra excited by ion bombardment differ significantly from spectra excited by electron bombardment. Low-energy spectra excited by electrons from metals generally show broad features roughly mirroring the self-convolution of the density of conduction band states. In contrast ion excited electron spectra in the same energy range contain sharp peaks, at any rate for some low-Z metals. This has been explained in terms of emission from excited species sputtered from the surface by the ion bombardment. The ion approaching the surface is neutralized before impact and the electron promotion model of Fano and Lichten [1] suggests that there is a high probability of neutral species in autoionizing states being produced in the collision. Thus the initial and final states involved in ion excited Auger (autoionizing) spectra are quite different from those involved in electron excited spectra, even in the case of free atom excitation. Ion excited Auger emission from solids is the subject of a recent review [2].

In addition to electron spectra from the target, peaks arising from the bombarding species can also be seen in the spectrum. Recent papers have reported the spectra of neon [3] and argon [4] produced by ion bombardment of silicon and aluminium substrates measured at high angular and energy resolution. These spectra contained considerable structure only previously seen in gas phase data and showed clear evidence of Doppler shifting due to Auger emission from moving atoms. The present paper reports measurements of the autoionizing spectra produced by the interaction of beams of Ar^+ and Ne^+ ions with energies in the range of 200 eV–5 keV with a magnesium surface.

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2. Experimental details

Details of the experimental apparatus are given in [3]. The energy of the electron beam used in the ion gun to ionize the rare gas was kept at 150 eV in the measurements reported here; this means that it was likely that some doubly ionized species were present in the ion beams.

The target was a 12 mm square piece of 99.99% pure Mg of thickness 1 mm. The target was mechanically abraded using fine-grain emery paper and then etched lightly in hydrochloric acid. The specimen was then mounted in a UHV chamber which was baked to 200 °C to reduce the base pressure to 3×10^{-10} mbar. Electron excited Auger electron spectroscopy (AES) showed that the surface was heavily contaminated with carbon, oxygen and chlorine. The surface was cleaned by rastering a 3 keV Ar^+ beam over the surface and the progress of the cleaning process was monitored at intervals with AES. After several hours bombardment the C and Cl signals had disappeared but O remained. The O peak remained unchanged for about 10 h but after that it gradually disappeared and the Mg metal signal emerged. The cleaning process was stopped when the O signal had merged with the background. The surface was continuously sputtered during measurement so once the surface was clean it remained clean thereafter. The target was biased by ~ -10 eV during measurements to increase the energy of the electrons in the analyser and so improve transmission.

Measurements were made with the ion beam incident at a glancing angle of $\sim 15°$ with the angle between the ion gun and the spectrometer optical axis fixed at 146°. The ion beam, optic axis and surface normal were coplanar in a horizontal plane. If the surface is considered to be planar, incident ions will be scattered at angles between 0° and 15°, so electrons entering the spectrometer will make angles between 4° and 19° with the direction of motion of the emitting rare gas ion.

3. Results and discussion

3.1. Argon and magnesium

Figure 1 shows the spectrum obtained when an Mg substrate is bombarded with 2 keV Ar^+ ions. The data are shown in the form recorded, with the energy shifted by a -10.6 V bias applied to the specimen and before background subtraction. The peaks numbered 1–6 arise from transitions in Ar while the peaks from Mg, labelled A–F, occur at higher energies and are well separated from the Ar peaks.

The shape of the spectrum is strongly dependent on incident ion energy. At low energies ($E <\sim 500$ eV) no Mg peaks were observed; as the energy was increased the Mg peaks grew until at ~ 1.5 keV the Mg and Ar peaks were of similar height. Further increase in energy resulted in a reduction of the Ar peaks; at 4 keV primary ion energy they were only just visible above the background and long recording times were required to obtain reasonable Ar spectra above this energy. Figure 2 shows this progression. The strong dependence of the low-energy Ar spectra on ion energy may explain why previous attempts to observe MNN spectra by Zampieri and Baragiola [5] were not successful, although they did make some measurements with incident energies below 1 keV without detecting an Ar spectrum.

The intensity of the Mg signal, normalized to unit ion beam current, was found to increase monotonically with incident ion energy. Vrakking and Kroes [7] found that the intensity of Auger emission from the target atoms varied as $(E_{in} - E_{th})^2$ and this relationship

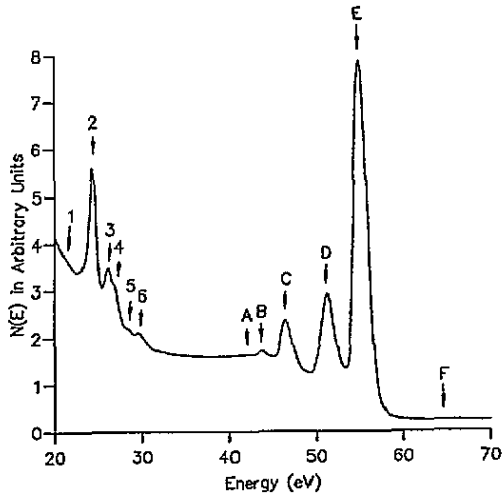

Figure 1. The electron spectrum obtained by bombarding Mg with 2 keV Ar^+ ions. Peaks 1–6 arise from Ar and peaks A–F from Mg. The data are as recorded, without background subtraction and with a 10.6 V bias applied to the specimen.

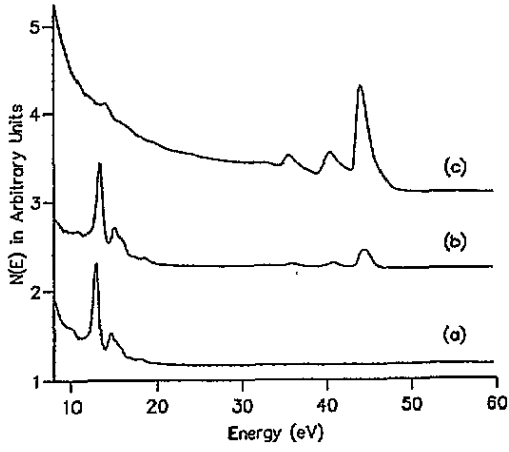

Figure 2. The variation of relative peak heights with incident Ar ion energy: (a) 500 eV; (b) 1 keV; (c) 5 keV.

was found to be reasonably well obeyed by our measurements. A least-squares fit to our data for peak E gave a value for the threshold energy, E_{th}, of (360 ± 50) eV in agreement with the value of 400 eV previously measured for Mg [7]. This is rather lower than recent measurements of the threshold by Mandarino *et al* [10] and may indicate the presence of small amounts of doubly ionized Ar. Peaks C and D showed similar behaviour with thresholds that could not be distinguished from that for peak E. Peak F behaved differently, with a threshold around 1600 eV, which is consistent with the observation that the peak could not be detected with 1600 eV primary ions. Vrakking and Kroes showed that the quadratic dependence of the emitted intensity on incident ion energy was consistent with a model of excitation of the target atoms by symmetrical target–target (T–T) collision processes. This

result has been confirmed by other authors for low-energy incident ions and is consistent with Monte Carlo simulations of the excitation process—see [2] for a discussion of this and a review of the literature. Recent careful measurements near the onset of target excitation by Mandarino *et al* [10] found that excitation with Ne^+ ions produced quite different results from excitation with Ar^+, Kr^+ and Xe^+. They concluded that the differences were due to contributions from asymmetrical projectile–target (P–T) excitation at low incidence energies present in the case of Ne bombardment but absent in the case of the other gases.

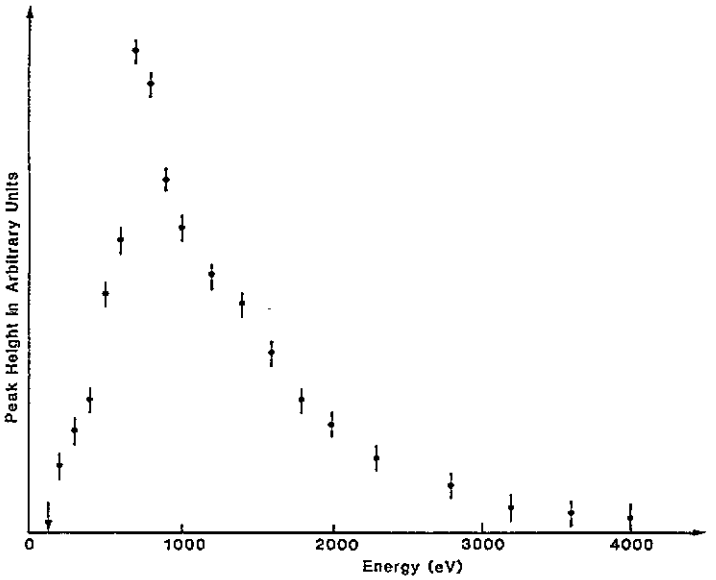

Figure 3. The normalized height of Ar peak 2 as a function of primary beam energy.

The energy dependence of the Ar Auger intensity is very different from that of Mg. The variation of the normalized height of Ar peak 2, identified as $3p^4 4s^2(^3P) \rightarrow 3p^5 + e$ transitions [4], with incident ion energy is shown in figure 3. The intensity initially rises very rapidly with incident ion energy but peaks at an incident energy estimated as (750 ± 30) eV and decreases with energy above this. The arrow on the energy axis of figure 3 indicates the threshold energy determined from measurements of the Doppler shift described below. Peak 3 ($3p^4 4s^2(^1D) \rightarrow 3p^5 + e$) follows a similar pattern. This behaviour is inconsistent with the Landau–Zener description, which predicts that beyond a critical energy and associated interatomic separation the probability of excitation is approximately constant. The results are, however, consistent with the data on $2p^4 3s^2(^1D) \rightarrow 2p^5 + e$ Ne transitions in Na^+–Ne collisions of Bydin and Godakov [11] and Olsen *et al* [12]. They attribute the resonant character of the cross-section to the gradual opening up of other competing channels, e.g. $2p^4 3s3p \rightarrow 2p^5 + e$. Although such higher excitations are indeed observed here, they do not appear to provide the compensation required. It is also important to note that the ^3P channel has greater intensity than the ^1D in our data in contrast to the case of closed shell–closed shell interactions, e.g. Na^+–Ne and Na^+–Ar, where symmetry inhibits the triplet channel. Previous work [2] suggests that at these incident energies the Ar^+ ions are neutralized prior to the collision; although the excitation may then be regarded as the result of a two-atom Ar–Mg collision, it would appear that the presence of the conduction electrons in the solid

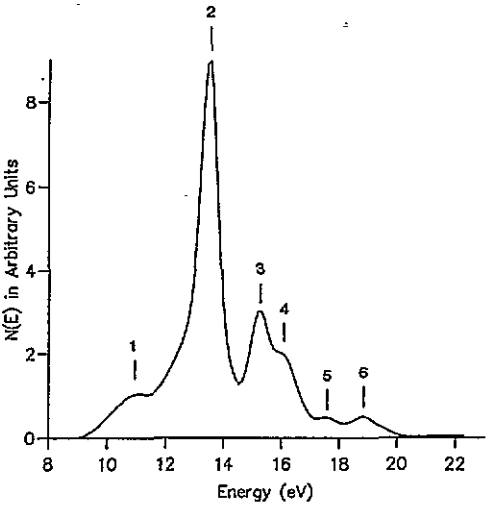

Figure 4. The Ar Auger spectrum recorded with 1 keV primary ions after removing a smooth background and correcting for the applied specimen bias.

allows the ^3P channel to flourish so that the relative intensities are now comparable with the respective channel statistical weights.

If a smooth background function is subtracted from the Ar spectra the fine structure can be readily seen (figure 4). Six peaks can be clearly resolved. The Ar spectra from Mg are similar to those from an Al rather than an Si target [4]: both the Al and Mg target spectra show two strong peaks, 2 and 3 in figure 4, and smaller peaks. However, the small peaks differ: in the case of Al the clearly resolved peak 4 in figure 4 is a barely distinguishable shoulder and there are three smaller peaks in the energy range occupied by peaks 5 and 6 in figure 4. A further difference is the presence of peak 1 in the data from Mg. This peak was very small or absent from the data from Al although it was strong in the Ar spectrum from an Si substrate, where many of the other small peaks could not be observed [4].

As in previous work the energies of the gas phase peaks were found to vary systematically with incident ion energy due to Doppler shift. In the case of Ne [3] a simple model was found to fit the data well. In this model, which is only applicable in the strongly forward scattering geometry used in these measurements, the measured energy E_m is related to the electron energy in the rest frame, E_A, by

$$E_m = E_A + (4m/M)^{1/2}\sqrt{E_A}\sqrt{E_I - E_L} \tag{1}$$

where m and M are the electron and ion masses and E_L is the energy lost by the argon ion in the excitation process. As in the case of the Ne data [3] we tried to fit a function of the form

$$E_m = E_A + k(E_I - E_L)^N. \tag{2}$$

The values of the adjustable parameters E_A, E_L, k and N obtained from a least-squares fit to the measured values of peak 2 are shown in table 1 together with the expected values based on equation (1). The measured values agree well with the predicted values although the estimated uncertainties are large in a number of cases: this is not entirely due to experimental

error; it also reflects the fact that the parameters in the model are highly correlated. The best value for the excitation energy, E_L, of $\sim$ 130 eV is consistent with our observation that the Ar signal became very weak for ion energies below 200 eV. The rest frame energy for peak 2 of 12.5 eV is relatively insensitive to the uncertainties in the values of the other parameters. Figure 5 shows a plot of the energy of peak 2 as a function of incident ion energy; the curve superimposed is the best fit of equation (2). The figure also shows the variation of the energy of peak 3; in spite of the similarity between the variation of peak 3 and that of peak 2 it proved impossible to fit equation (2) to these data, presumably because of the greater errors in determining the exact position of the smaller peak. In the case of Ar on Al a fit to equation (2) could only be obtained for ion energies lower than 500 eV [4].

Table 1. *Measured and calculated parameters for the simple Doppler model applied to Ar—* equation (2) in the text.

	E_A (eV)	k $(eV)^{1/2}$	E_L (eV)	N
Argon peak 2	12.47 ± 0.05	0.03 ± 0.04	130 ± 170	0.51 ± 0.14
Calculated values		0.026	<200	0.50

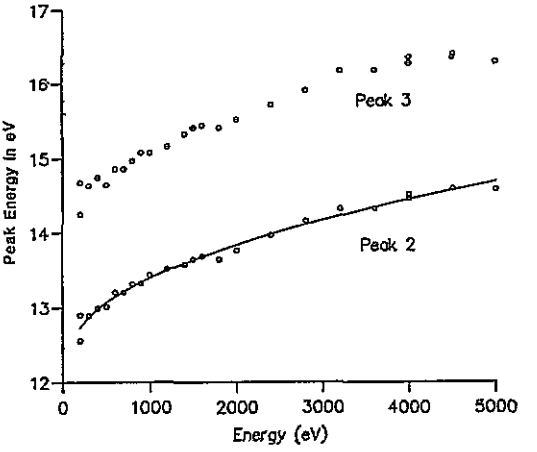

Figure 5. The variation of the energies of peaks 2 and 3 in the Ar Auger spectrum. The smooth curve is the least-squares fit of equation (2) to the data. No fit could be obtained for peak 3.

The Mg peaks were also measured as a function of incident ion energy but no systematic variation with energy was found and it was concluded that the Mg peaks are not Doppler shifted to within an uncertainty of $\sim$ 0.1 eV. If the Mg peaks recorded with high-energy ions are compared with those recorded with a lower ion energy, a tailing of these peaks towards higher energies could be seen and this could well be caused by a Doppler broadening due to a small increase in the energy spread of the emitting Mg atoms.

The Doppler model may be used to determine the rest frame energies of the Ar peaks for each incident ion energy. This was done for a set of 25 measurements spanning a range of incidence energies from 200 eV to 5 keV. The best-fit parameters given in table 1 were used in equation (2). The results are shown in table 2. The uncertainties quoted are the

Table 2. Measured values of the Ar peaks shown in figure 3. The Doppler model has been used to refer all energies to the rest frame. Calculated values and measured values from Al and Si targets are quoted from [4]. All energies are in electronvolts. In the case of the calculation, the two values indicate the width due to multiplet structure

	1	2	3	4		5	6
This work	10.1	12.5	14.1	14.9		16.4	17.6
±	0.5	0.07	0.10	0.08		0.10	0.07
Nixon *et al* [4]							
Al target	8.7?	12.0	13.8	14.5	15.3	16.0	16.8
Si target	9.9	11.8	13.9		15.2		
Calculated values							
Initial state							
$(\ )3p^4 4s^2$		11.3	13.4				17.4
		^3P	^1D				^1S
$(\ )3p^4 4s^1 4p^1$		11.8	13.9			16.0	
		12.9	14.6			16.0	
$(\ )3p^4 3d^1 4s^1$		11.7	12.5	15.3		16.1	17.1
		11.9	14.7	15.7		16.5	17.8

standard deviations of the distributions. Also shown in table 2 are the values for the peaks from an Al substrate measured by Nixon *et al* [4] and the energies predicted by them using the Dirac–Fock program of Grant [6] based on transitions from excited states in neutral Ar to the $3s^2 3p^5$ ground state of the Ar^+ ion. The agreement with the Al data is good for peaks 2–5; there appears to be a small systematic shift, which can be ascribed to work function differences. Candidates for most of the peaks can be found in the calculated values, which span quite wide ranges because of multiplet effects.

Peak 1 is a problem. This peak shifts systematically with ion energy, appearing at about 10.0 eV in the low-energy ion data and shifting to about 12.9 eV at ion energies in the 4.5–5 keV range. This shift is actually larger than the Doppler shift in peaks 2–6 and this is the reason for the large standard deviation about the mean energy for this peak; the shift with incident ion energy would seem to eliminate the possibility of emission from ions embedded in the solid or from slow excited neutrals. The peak is broad and difficult to measure accurately but the systematic shift is clearly established by the data. Brenton *et al* [8] suggested that such a peak might arise due to decay of a temporary negative Ar ion. However, in this case it is not clear why the energy dependence of such a peak would differ from that of the other Ar peaks.

The Mg spectrum is shown in figure 6 with six peaks visible. Peaks E, D, C and F correspond to the peaks labelled I, II, III and IV by Whaley and Thomas [13], who used 140 keV ions to produce their spectra; peaks A and B are new features. 'Three-peak' structures similar to the data of Whaley and Thomas have been reported by Saiki and Tenaka [14] using 5–10 keV Ar ions and by Milne and Fabian [15], who used 10 keV caesium ions to excite their spectra. The variation of peak F (IV) with incidence energy is quite different from the other peaks. Peaks A–E grow together in intensity with increase in incident ion energy with a threshold $\sim$ 400 eV but peak F could not be detected at incidence energies below 1800 eV; the data recorded in figure 6 at 2 keV are just above threshold. This peak is prominent in the data of Whaley and Thomas [13] but absent from the spectrum of Milne and Fabian [15], who concluded that the initial state responsible for

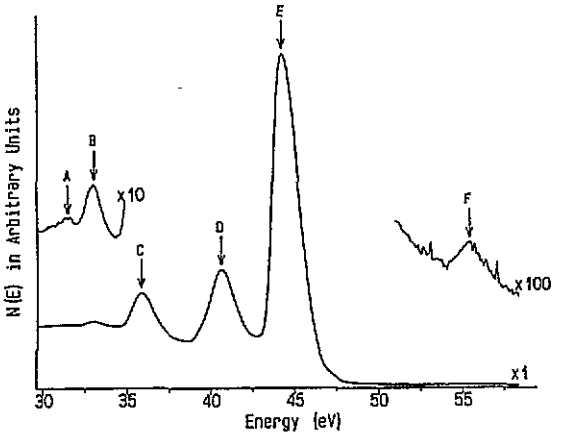

Figure 6. The Mg Auger spectrum excited with 2 keV Ar ions.

this transition could not arise from T–T interaction but must be excited by P–T processes. A similar conclusion was reached by Xu *et al* [16] based on the analysis of the variation of this peak with incident energy. Similar peaks are found in Al and Si spectra and are believed to arise from autoionizing states of singly charged metal ions with two vacancies in the 2p level (see [16]).

Table 3. Measured values of the Mg peaks labelled as in figure 6 together with estimates of the energies based on de-excitation from a common initial state. The measured values and assignments from Whaley and Thomas are given for comparison. All energies are in electronvolts.

	A	B	C	D	E	F
This work	31.2	32.8	35.6	40.3	43.9	55.3
±	0.3	0.2	0.2	0.2	0.2	0.2
Final configuration						
($1s^2 2s^2 2p^6$)	5s,4d	4p	4s	3p	3s	
	4f,5p		4d			
Calculated Energy	31.8	33.9	35.0	39.5	43.9	
	−32.4	−34.6	−35.9	−40.2	−44.6	
			III	II	I	IV
Whaley and Thomas [13]			34	39	43	54
Transition [13]			$2p^5 3s^2$	$2p^5 3s^2 3p$		
			$-2p^6(^1S)$	$-2p^6 3s(^2P)$	$-2p^6 3s(^2S)$	

The energies of peaks A–F are shown in table 3 together with the values obtained by Whaley and Thomas. The peaks I–IV were indexed by Whaley and Thomas, following Dahl *et al* [17], as arising from excited initial states in Mg^0 (peaks E and D) and Mg^+ (peaks C and F); their labels are shown in table 3. While the behaviour of peak F with incidence energy strongly suggests a different origin from the other peaks there seems no obvious reason for assigning peaks E, D and C to different ionic species; indeed the additional peaks B and A appear to fit in a series with the other peaks. The variation in relative intensities with incidence energy shows no systematic variation over the range

1–4.5 keV and the measured ratio of 1:0.2:0.1 is very similar to the ratio measured from the graph published by Whaley and Thomas [13] (they quote F:D as 1:0.2). Perhaps more significantly, the same ratio of intensities is obtained from the published spectrum of Milne and Fabian [15], who produced their spectra by bombardment with 10 keV Cs^+ ions.

While not conclusive evidence, this suggests that it might be reasonable to look for labels in terms of transitions from a single excited state in Mg^0 decaying to a series of excited states above the ground state. Such a series is suggested in table 3; the common initial configuration is $1s^22s^22p^53s^23p$ in neutral Mg and the lowest state to which this decays after electron emission is the ground state configuration of Mg^+, $1s^22s^22p^63s$. The difference in energy is given by Dirac–Fock calculation as 43.9–44.6 eV, in close agreement with the Hartree–Fock calculation quoted by Dahl *et al* [17]. The transition to the ground state is assigned to the most intense feature E. The energies of the excited configurations above the ground state in Mg^+ can be obtained from Moore [18] and hence transition energies to these configurations can be obtained. In this way reasonable candidates can be obtained for peaks A, B, C, D and E as shown in table 3.

3.2. *Neon and magnesium*

The Ne^+ excited spectrum contains more structure than that obtained with Ar^+. Figure 7 shows the spectrum produced by 4.0 keV Ne^+ ions: the peaks marked 1–12 arise from transitions in Ne while those marked B–F arise from Mg and correspond to the peaks with the same labels in the Ar^+ induced spectrum (figure 1). The overlap between the Mg and Ne peaks makes measurement of the smaller Mg peaks impossible but peaks C, D and E were measured at 35.7 eV, 40.4 eV and 43.9 eV in good agreement with the values measured with Ar^+ excitation. The peak F could only be observed with incident energies of 3 keV and above and even at 5 keV it was very weak. However, it was intense enough to be measured after background subtraction and a value of 55.2 eV was obtained, again in agreement with measurements of the Ar^+ excited data.

The incident ion energy dependence is different from the case of Ar^+ ions. At the lowest energies where spectra are detectable, $\sim$ 200 eV, only Ne peaks are present. At energies $\sim$ 300 eV the Mg peaks begin to emerge and as the energy of the incident beam increases both sets of peaks grow in prominence. At the highest incidence energies used, up to 5.0 keV, the Mg peaks were still considerably less intense than those of Ne. The sequence is illustrated in figure 8; the Doppler shift can also be clearly seen in this figure. The Ne peaks shift to higher energies with primary energy while the Mg peaks remain at constant energy. The behaviour of the Ne intensities with incidence energy is similar to that described by Ferante and Pepper [19], who reported a sharp rise followed by a broad maximum in the intensity against energy curve for Ne^+/Mg and Ne^+/Al. The variation of Mg peak E with incident ion energy again fitted the quadratic model of Vrakking and Kroes [7].

The variation of the energies of peaks 3 and 5 with incident ion energy fitted the Doppler model well. The best-fit parameters for the most intense peak, peak 3, could be used to determine the rest frame peak energies for each of the primary beam energies used. This gave the averaged rest frame energy of peak 5 as (23.81 ± 0.08) eV. Andersen and Olsen [9] measured this peak at 23.55 eV in their gas phase data using a calibration method that could be referred back to optical data. This gives a difference of 0.26 eV to account for work function differences and calibration error. This value has been subtracted from all of the peak energies quoted above. As in the case of Ar^+ excitation no systematic shift in the Mg peaks with primary energy could be detected and it is concluded that Doppler shifts, as

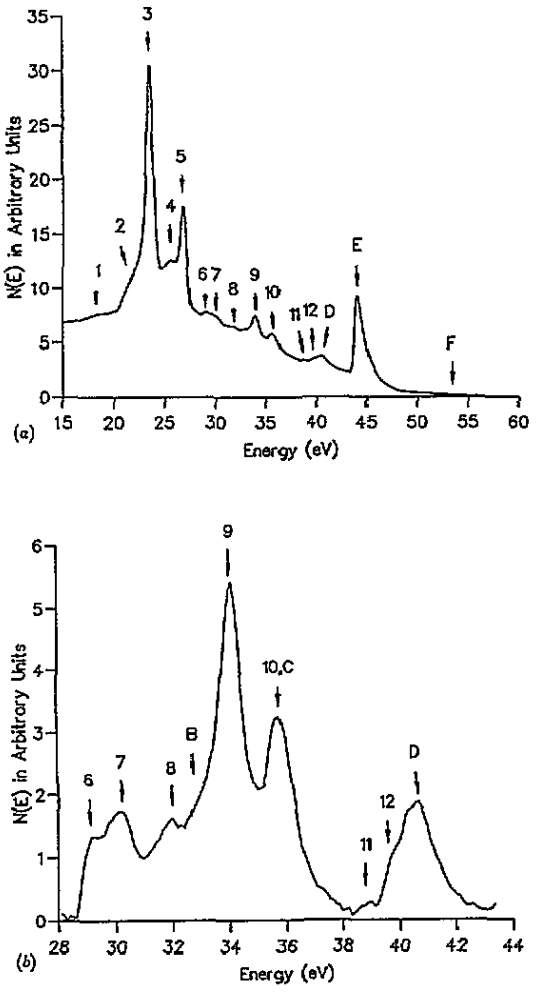

Figure 7. (a) The spectrum obtained by bombarding an Mg target with 4 keV Ne^+ ions. Peaks 1–12 arise from transitions in Ne. (b) Part of the curve at increased gain and with a smooth background subtracted.

opposed to Doppler broadening, are absent from the Mg spectra in the range of ion energies used here.

The low-energy end of the Ne spectrum again shows differences from that obtained from an Al target in that two peaks, 1, at (15.1 ± 0.3) eV, and 2, at (18.7 ± 0.4) eV, were detected below the most intense peak, 3. These peaks were of low intensity and relatively broad but they could easily be measured. Unlike the similar peak in the Ar spectrum, they fitted the Doppler model quite well and no systematic deviations were detected with increasing energy. No definite identification is proposed for these peaks beyond the possibilities already mentioned for Ar.

4. Conclusions

The Ne and Ar autoionizing spectra obtained when an Mg substrate is bombarded with Ne^+

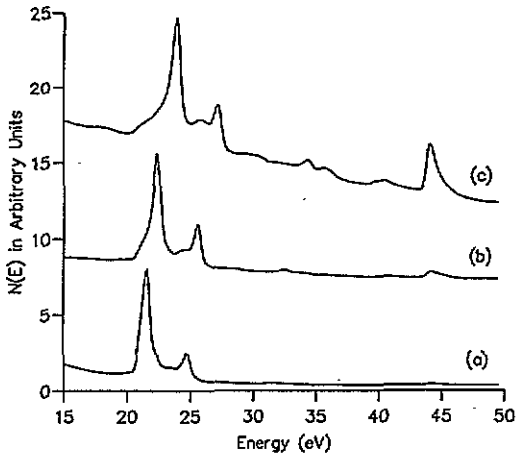

Figure 8. The Ne and Mg spectra recorded with different incident ion energies: (a) 600 eV; (b) 1.5 keV; (c) 5.0 keV.

and Ar^+ ions with energies in the range 300–5000 eV contains considerable structure. In the case of neon this structure is very similar to that obtained with an Al target except for the presence of two small low-energy peaks. The Ar spectrum from Mg also showed a low-energy peak not present in the case of an Al substrate and the structure of the smaller peaks also showed clear differences from the data recorded with an Al target. The variation of height of the principal peaks with incident ion energy showed very different behaviour, with Ar giving a sharp peak at low energy; this behaviour was not found with Ne and Mg.

New structure was observed at the lower end of the Mg spectrum and it was concluded that the five peaks measured in the range 30–45 eV formed a series. These peaks could be indexed as arising at transitions from an excited state in neutral Mg to the ground state and states above the ground state in Mg^+. This contrasts with previous explanations, which assigned these peaks to transitions from both Mg^0 and Mg^+ initial states.

The simple Doppler model appropriate to the glancing incidence geometry employed here fitted both sets of data reasonably well. This model was used to determine the rest frame energies of the measured data and these data were found to be consistent with theoretical predictions based on the decay of excited autoionizing states in the neutral rare gas atoms. No Doppler shift was measured for the Mg peaks and it is concluded that the excited Mg atoms are sputtered with low kinetic energies.

Acknowledgments

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References

[1] Fano U and Lichten W 1967 *Phys. Rev.* **14** 627
[2] Valeri S 1993 *Surf. Sci. Rep.* **17** 85
[3] Gallon T E and Nixon A P 1992 *J. Phys.: Condens. Matter* **4** 9761

[4] Nixon A P, Gallon T E, Yousif F and Matthew J A D 1994 *J. Phys.: Condens. Matter* **6** 2681
[5] Zampieri G and Baragiola R A *1986 Phys. Rev.* B **33** *588*
[6] Grant I P 1972 *Comput. Phys. Commun.* 9 377
[7] Vrakking J and Kroes A 1979 *Surf. Sci.* **84** 153
[8] Brenten H, Muller H, Niehaus A and Kempter V 1992 *Surf. Sci.* **278** 183
[9] Olsen J O and Andersen N 1977 *J. Phys. B: At. Mol. Phys.* **10** 101
Andersen N and Olsen J O 1977 *J. Phys. B: At. Mol. Phys.* **10** L719
[10] Mandarino N, Zoccali P, Oliva A, Camarca M, Bonanno A and Xu F 1993 *Phys. Rev.* A **48** 2828
[11] Bydin Yu F and Godakov S S 1976 *Pis. Zh. Eksp. Teor. Fiz.* **23** 566 (Engl. transl. 1976 *JETP Lett.* **23** 518
[12] Olsen J O, Andersen T, Barat M, Courbin-Gaussorgues Ch, Sidis V, Pommier J, Augusti J, Andersen N and Russek A 1979 *Phys. Rev.* A **19** 1475
[13] Whaley R and Thomas E W 1984 *J. Appl. Phys.* **56** 1505
[14] Saiki K and Tanaka S 1984 *Nucl. Instrum. Methods Phys. Res.* B **2** 512
[15] Milne R H and Fabian D J 1991 *Appl. Phys.* A **53** 574
[16] Xu F, Mandarino P, Zoccali P, Calaminici P, Oliva P and Bonanno A 1993 *Phys. Rev.* B **48** 9987
[17] Dahl P, Rodbro M, Hermann G, Fastrup B and Rudd M E 1976 *J. Phys. B: At. Mol. Phys.* **9** 1581
[18] Moore C E 1949 *National Bureau of Standards Circular* 476
[19] Ferrante J and Pepper S V 1976 *Surf. Sci.* **57** 420