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Screening of core holes in Al-Mg alloys studied by a comparison of KL_1V and $KL_{2,3}V$ Auger spectra

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The Mg and Al KL_1V and $KL_{2,3}V$ Auger profiles are measured for Al-Mg alloys and compared with the soft-x-ray profiles of similar materials. A comparison of the elemental KL_1V and $KL_{2,3}V$ profiles reveals the contribution made to the screening of a core hole by the s partial density of states (PDOS). In the pure elements and on Al sites in Al-Mg alloys, the core hole induces a peak at the bottom of the band in the s PDOS. This does not happen on Mg sites in dilute Mg alloys. This difference in core-hole screening on Mg and Al sites in the alloys is explained in terms of the difference in core charge between the local core-ionized site and an average lattice site.

INTRODUCTION

The spectral profiles of core-core-valence Auger transitions in simple metals have been shown[1–3] to yield information about the local partial densities of states (PDOS) around a core-ionized atom. In particular it is known that the presence of the core hole distorts the local s PDOS and causes a peak to appear at the bottom of the band.[1–7] However, the shape of the local p PDOS is almost unchanged by the presence of the core hole. The profiles of $KL_{2,3}V$ transitions, which are dominated by matrix elements involving the p PDOS, rise rapidly with increasing binding energy from the top of the band, reach a peak just below the Fermi energy, and then fall away smoothly towards the bottom of the band. However, the KL_1V transitions, which have roughly equal contributions from the s and p PDOS, have spectral profiles which show a double peak structure with the peak- to high-binding energy arising from a feature induced at the bottom of the s PDOS by the presence of the core hole.

In alloys between Mg and noble or transition metals we have shown[8,9] that the presence of the d band of the other alloy constituent gives rise to additional peaks in the spectral profiles of the Mg KL_1V and $KL_{2,3}V$ transitions. These additional peaks arise from the hybridization of the Mg s and p PDOS with the transition- or noble-metal d band.[8,9] In Mg-Zn alloys the Zn d band does not induce additional peaks in the Mg KL_1V and $KL_{2,3}V$ spectral profiles[8,9] probably because the Zn d band is too tightly bound to hybridize with the Mg s and p PDOS and indicating that Mg-Zn alloys should be regarded as alloys between simple metals. It has also been observed[9] that the peak in the Mg KL_1V spectrum associated with the bottom of the Mg s PDOS decreases in intensity with increasing Zn content so that the Mg KL_1V profile comes to resemble the Mg $KL_{2,3}V$ profile. The same behavior was observed[9] in the Mg Auger profile of Al-Mg alloys and this suggests that in alloys between simple metals the presence of a core hole does not always induce a peak at the bottom of the band in the local s PDOS. In this work we study both the Mg and Al KLV Auger profiles of Al-Mg alloys. We show that a core hole on a Mg site in an alloy with a low Mg content (denoted *Al*Mg) is not screened by a distortion of the local s PDOS whereas a core hole on an Al site in an alloy with a low Al content (denoted Al*Mg*) is screened by a distortion of the local s PDOS. This asymmetric behavior is reconciled with the idea of a common band for the conduction electrons of Al-Mg alloys by consideration of the different valence of the constituents.

EXPERIMENTAL

Auger and photoelectron spectra were measured with a modified Kratos ES200 photoelectron spectrometer equipped with a multidetector.[10] The spectrometer is fitted with a monochromated Al $K\alpha$ x-ray source and with two Henke x-ray guns giving a choice of Al $K\alpha$ or Si $K\alpha$ characteristic x rays. The Mg Auger spectra and photoelectron spectra of the valence bands and core levels of the alloys were excited with Al $K\alpha$ x rays and the Al Auger spectra were excited with Si $K\alpha$ x rays. The spectrometer was pumped by ion pumps and titanium sublimation pumps and these experiments were conducted in pressures of $< 10^{-9}$ Torr.

Al-Mg alloys were made by cosputtering the two elements onto a Cu substrate, the compositions being determined by the relative intensities of Al and Mg core-level photoelectron lines as described earlier.[8,9] To characterize the specimens, we studied the energy loss accompanying the core-level photoelectron lines. The energies and widths of plasmons observed from our specimens agreed with the results of measurements on bulk specimens of similar composition[11–13] indicating that the cosputtered specimens adopted the equilibrium phase structure appropriate to their compositions.[14] The alloys studied here are expected to be of mixed phase. However, since the Auger profiles depend only on the immediate local environment and not on the crystal structure, the presence of two phases in the specimens is not significant.

RESULTS

Mg and Al *KLV* Auger spectra

The aim of this work is to understand the changes in the local *s* and *p* PDOS around core-ionized Mg and Al atoms brought about by alloying. These PDOS have a strong influence on the *KLV* Auger profiles and the most interesting information should be obtained from studies of dilute alloys, *Al*Mg and Al*Mg*, where an atom of one metal is almost entirely surrounded by atoms of the other constituent. Consequently we concentrate on the alloys $Al_{85}Mg_{15}$, a mixture of the α and β phases and Al_8Mg_{92}, a mixture of the γ and δ phases.

The profiles of *KLV* Auger transitions may be used to show the *s* and *p* PDOS around a core-ionized site. The energy scales for these valence-band densities of states (DOS) are obtained from the kinetic energies of the Auger spectra $E^F_{\text{kin}}(KLV)$ and the binding energies of the core levels $E^F_B(K)$ and $E^F_B(L)$ measured in x-ray photoemission spectroscopy (XPS) using

$$E^F_B(V)=E^F_B(K)-E^F_B(L)-E^F_{\text{kin}}(KLV)\ , \qquad (1)$$

where all the quantities are referenced to the Fermi energy. The assumptions implicit in the use of Eq. (1) are discussed in an earlier paper.[8]

According to the final-state rule[2,7,15,16] the profiles of *KLV* transitions will reflect the *s* and *p* PDOS around the core-ionized site modified by matrix-element effects. The matrix elements which cause the $KL_{2,3}V$ spectra to be dominated by the *p* PDOS and the KL_1V spectra to show roughly equal contributions from the *s* and *p* PDOS are not expected to introduce any additional structure into the Auger profile.[2,17] Calculations indicate that for elemental metals the presence of a core hole does not change the shape of the local *p* PDOS but it does introduce a strong peak in the *s* PDOS at the bottom of the band. The pres-

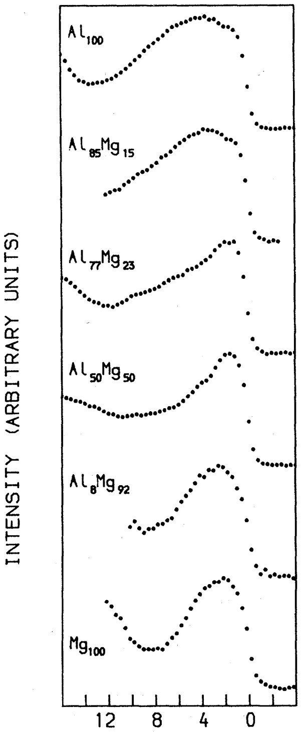

FIG. 1. The valence-band photoelectron spectra of Al-Mg alloys.

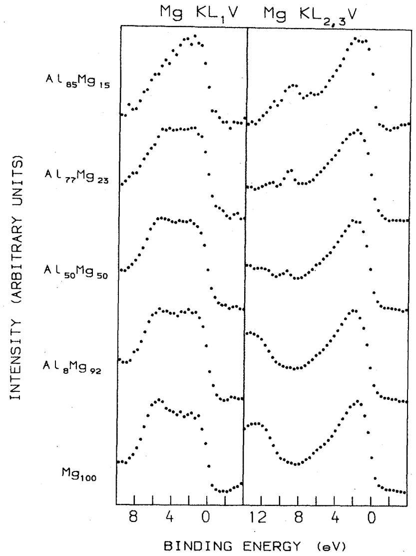

FIG. 2. The Mg KL_1V and $KL_{2,3}V$ Auger spectra of Al-Mg alloys. The results for $Al_{77}Mg_{23}$ and $Al_{50}Mg_{50}$ are from Davies and Weightman (Ref. 9). The Mg $KL_{2,3}V$ of the dilute Mg alloys show features at a binding energy of $\sim$9 eV which arise from the photoelectron spectrum of Ar adsorbed during specimen manufacture. The intensity of these features indicates an Ar level of $<1\%$ of the Mg concentration (Ref. 8).

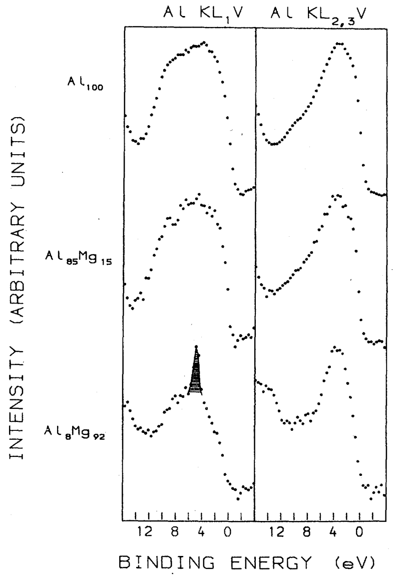

FIG. 3. The Al KL_1V and $KL_{2,3}V$ Auger spectra of Al-Mg alloys. The shaded feature in the KL_1V spectrum of Al_8Mg_{92} results from the Mg 2*p* photoelectron line excited by Al $K\alpha$ x rays generated in the specimen.

ence of the core hole is not expected to have a significant effect on the width of the valence band.

Alloying will have an effect on the width of the valence band and this can be seen in the valence-band *XPS* spectra of Fig. 1. It is difficult to determine the width of the valence band accurately due to the contribution made by energy-loss processes. The valence-band *XPS* spectrum of pure Mg has been shown[18] to be consistent with the width of ~ 7.0 eV expected from band-structure calculations and the spectra of Fig. 1 show that the valence-band width of Al_8Mg_{92} is very similar. The valence-band *XPS* spectra of the two Al-rich alloys show differences in shape from that of pure Al but all three materials have a width of ~ 11.5 eV consistent with that expected from band-structure calculations for pure Al.[19]

The Mg KLV spectra of pure Mg and Al-Mg alloys are shown in Fig. 2. Figure 3 shows the Al KLV spectra of pure Al and the Al-Mg alloys. The presence of energy-loss contributions makes it difficult to determine the widths of these spectral profiles. However like the valence-band *XPS* spectra (Fig. 1) the widths of the KLV Auger profiles are consistent with the idea that in the alloys the Al and Mg conduction electrons occupy a common band with a width intermediate between that of the pure elements. The narrowness of the Al KLV spectra for Al_8Mg_{92} (Fig. 3) is suggestive of this interpretation.

The shape of the Mg $KL_{2,3}V$ spectrum is dominated by the local p PDOS around a core-ionized Mg site and the spectral profiles of these transitions observed from pure Mg and Al_8Mg_{92} are almost identical showing that the addition of a small amount of Al does not change the local p PDOS around a core-ionized Mg site. The Mg $KL_{2,3}V$ spectra observed from more dilute *Al*Mg alloys show photoelectron lines from Ar absorbed during manufacture of the specimens. These spectra obscure the low-energy region of the Mg $KL_{2,3}V$ profiles. However, the presence of the small amount of absorbed Ar indicated by the photoelectron peaks in Fig. 2 should not affect the DOS around a Mg or Al site. The KLV transitions are weak features and the levels of Ar contamination shown in Fig. 2 correspond to Ar concentrations of $\sim 1\%$ of the Mg concentration.[8] In the *Al*Mg specimens the Mg $KL_{2,3}V$ profiles show a broadening near the peak but apart from this the spectra indicate that the local p PDOS around a core-ionized Mg site is very similar to that in pure Mg.

The Mg KL_1V Auger profiles are also shown in Fig. 2. These show striking variations in shape with composition. The KL_1V profile is made up of roughly equal contributions from the local s and p PDOS around a core-ionized site. This accounts for the double-peaked structure of the pure Mg KL_1V profile: the peak just below E_F arises from the p PDOS which dominates the $KL_{2,3}V$ profile and the peak- to high-binding energy arises from the feature induced at the bottom of the band in the s PDOS by the core hole. The spectra show that the addition of only 8% of Al is sufficient to reduce the prominence of the peak in the s PDOS in the $KL_{2,3}V$ profile. The spectra of Fig. 2 show that as the Al content if increased it becomes harder to discern the peak in the s PDOS. For $Al_{85}Mg_{15}$ this feature has disappeared and the Mg KL_1V profile looks similar to the Mg $KL_{2,3}V$ profile.

The KL_1V and $KL_{2,3}V$ Auger profiles of Al excited by Si $K\alpha$ x rays are shown in Fig. 3. The Al KL_1V spectrum of the alloys is overlapped by the Mg $2p$ *XPS* line excited by Al $K\alpha$ x rays generated in the specimen. This internal *XPS* line, shown shaded in Fig. 3, is always present in the electron spectra of Al-Mg alloys but the Al $K\alpha$ and KLV transition rates and the Mg $2p$ photoelectron cross section are such that the peak only has significant intensity, compared to the Al KL_1V spectrum, for Al*Mg* alloys (Fig. 3, Al_8Mg_{92}). The Al KL_1V and $KL_{2,3}V$ profiles of $Al_{85}Mg_{15}$ are similar to those of pure Al. This suggests that the local s and p PDOS around a core-ionized Al is unchanged by alloying with low levels of Mg. For the dilute alloy Al_8Mg_{92} the Al $KL_{2,3}V$ and KL_1V spectra are much narrower than in pure Al and have a width similar to that of the pure Mg bandwidth (Fig. 1).

The changes in the Mg and Al KLV Auger caused by alloying can be clearly seen in Fig. 4. The left-hand panels compare the profiles of the Mg KL_1V and $KL_{2,3}V$ spectra in pure Mg and $Al_{85}Mg_{15}$. The difference between the two profiles, shown by the diagonal shading, is mainly due to the greater importance of the s PDOS in the KL_1V profile. The figure shows that this difference between the Mg Auger profiles is pronounced in pure Mg but has almost disappeared in $Al_{85}Mg_{15}$. The right-hand panels show a similar comparison for the Al Auger spectra. For

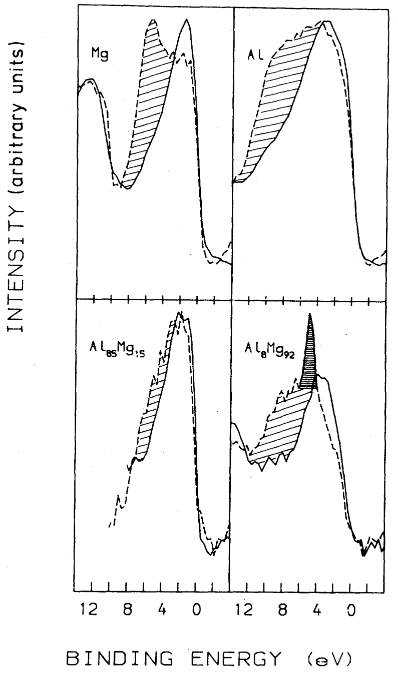

FIG. 4. The full lines show $KL_{2,3}V$ spectra and the dashed lines KL_1V spectra. The diagonal shading shows the difference between these profiles. The top panels show a comparison of the KL_1V and $KL_{2,3}V$ spectra of the pure metals. The bottom left panel compares the Mg KL_1V and $KL_{2,3}V$ of $Al_{85}Mg_{15}$. The bottom right panel is a comparison of the Al KL_1V and $KL_{2,3}V$ spectra of Al_8Mg_{92}. The horizontal shading in this latter figure is an internal photoemission line which overlaps the Al KL_1V spectrum.

the Al_8Mg_{92} alloy the comparison is complicated by the superposition of the internal photoemission peak, shown horizontally shaded, on the Al KL_1V spectrum. However, Fig. 4 makes it clear that the energy dependence of the *s* PDOS around a core-ionized Al site in an Al*Mg* alloy is similar to that around a core-ionized site in pure Al.

Comparison with soft x-ray spectra

For the pure simple metals, Na, Mg, and Al, the shapes of *KLV* Auger profiles (Fig. 4) have been reconciled with the profiles of *KV* and $L_{2,3}V$ soft-x-ray spectra.[2,3,6] This synthesis,[1–7,17] which we term the standard model, rests on a number of assumptions and expectations:

(1) Although the matrix elements for x-ray and Auger processes are dependent on the angular momentum of the valence-electron DOS they vary smoothly with energy across the band so that the spectral profiles reflect the shape of the local valence-band densities of states for each angular momentum component.

(2) The shapes of the valence-band DOS are determined by the final-state rule so that soft x-ray spectra show the profile of the local DOS around a neutral atom while *KLV* spectra show the local DOS around a core-ionized atom.

(3) Within a given environment, and to the extent that differences in lattice spacing can be ignored, the equivalent-cores approximation may be used to equate the shapes of the local valence-band DOS around a neutral atom of atomic number *Z* with that around a core-ionized atom of atomic number $Z-1$.

(4) The presence of a core hole is expected to generate a peak at the bottom of the band in the *s* PDOS but not to distort the shape of the *p* PDOS.

We have recently shown that the Mg *KLV* Auger spectra of alloys of Mg with transition and noble metals can also be understood within the standard model,[8,9] additional peaks in the *KLV* profiles arising from the hybridization of the Mg *s* and *p* PDOS with the *d* band of the other alloy constituent.

We now examine whether the *KLV* Auger spectral profiles of Al-Mg alloys can be reconciled with the standard model. By the equivalent-cores approximation we expect the DOS around a core-ionized Mg site in an environment of Al atoms to be the same as that around an Al site in pure Al. This expectation is borne out for the *p* PDOS by the agreement in shape of the Al *KV* x-ray profile from pure Al with the Mg $KL_{2,3}V$ Auger profile of $Al_{85}Mg_{15}$ [Fig. 5(a)]. In order to test whether the standard model also works for the *s* PDOS we compare the Al $L_{2,3}V$ x-ray profile from pure Al with the Mg KL_1V spectrum of $Al_{85}Mg_{15}$ [Fig. 5(b)]. The Al $L_{2,3}V$ x-ray profile shows a peak at the Fermi level which arises from the many-body response of the conduction electrons due to the change in potential caused by the creation of the core hole. Since core holes are present in both the initial and final states of the *KLV* processes no such many-body response is expected[2] and there is no corresponding peak in the Auger spectrum. The Al $L_{2,3}V$ profile should show the *s* PDOS around an Al site in an Al environment while the Mg KL_1V profile of $Al_{85}Mg_{15}$ will be made up of roughly equal contributions from the *s* and *p* PDOS around a core-ionized Mg site in an Al environment. Figure 5(b) shows that the two profiles differ at the bottom of the band. The standard model leads one to expect significant intensity in the *s* PDOS at the bottom of the band in the Mg KL_1V spectrum. This is not observed and it indicates that the *s* PDOS around a core-ionized Mg site in $Al_{85}Mg_{15}$ is quite different from that around an Al site in pure Al: For this case the standard model fails.

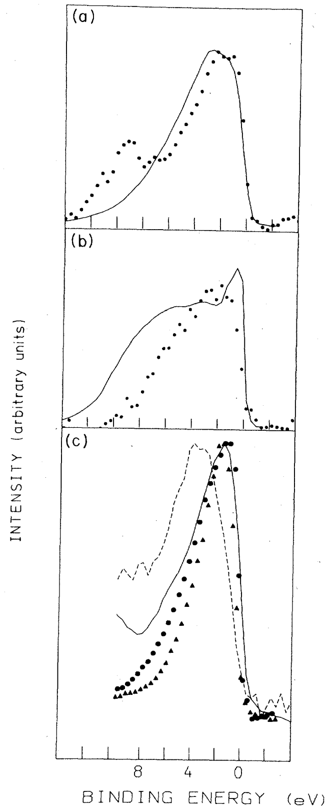

FIG. 5. (a) The full line shows the *KV* x-ray profile of pure Al (Ref. 20). The dots show the Mg $KL_{2,3}V$ Auger profile of $Al_{85}Mg_{15}$. Superimposed on the Auger profile at a binding energy of ~9 eV are photoelectron lines from adsorbed Ar. (b) The full line shows the $L_{2,3}V$ x-ray profile of pure Al (Ref. 20). The dots show the Mg KL_1V Auger profile of $Al_{85}Mg_{15}$. (c) The triangles show the *KV* x-ray profile of pure Mg (Ref. 20) and the full line shows the $KL_{2,3}V$ Auger profile of pure Mg. The circles show the Al *KV* x-ray profile of Al_5Mg_{95} (Ref. 20) and dashed line shows the Al $KL_{2,3}V$ Auger profile of Al_8Mg_{92}. By the final-state rule these profiles are dominated, respectively, by the *p* PDOS around neutral Mg, core-ionized Mg, neutral Al, and core-ionized Al sites all in a Mg environment. These correspond to differences ΔZ between the core charges of the local site and average sites of 0, +1, +1, and +2, respectively.

We cannot test the standard interpretation for the Al *KLV* spectra in the dilute Al alloys since the equivalent-cores model would liken the *s* and *p* PDOS around a core-ionized site in Al-Mg to the $L_{2,3}V$ and *KV* x-ray profiles of Si in Mg-Si alloys and we do not know of such x-ray data. However, we can test the extent to which the p PDOS around a site is insensitive to the difference between the core charge on that site and on a normal site. We term this difference ΔZ. Figure 5(c) shows a comparison of the spectral profiles of Mg KV x rays from pure Mg,[20] the Mg $KL_{2,3}V$ Auger profiles of pure Mg, the Al KV x-ray profile from $\mathrm{Al_5Mg_{95}}$,[20] and the Al $KL_{2,3}V$ Auger profile of $\mathrm{Al_8Mg_{92}}$. These correspond, respectively, to the p PDOS around a neutral Mg ($\Delta Z=0$), a core-ionized Mg ($\Delta Z=+1$), a neutral Al ($\Delta Z=+1$), and a core-ionized Al ($\Delta Z=+2$) all in a Mg environment. The agreement between the two $\Delta Z=+1$ measurements supports the standard model. Figure 5(c) shows that whereas a difference in core charge of $+1$ between the site being probed and a normal site only causes a slight broadening of the local p PDOS the larger $\Delta Z=+2$ difference does pull the p PDOS towards the bottom of the band. One would anticipate that for a sufficiently large ΔZ a bound state would be formed.

DISCUSSION

The most striking conclusion from this study is the confirmation[9] that the core ionization of a Mg site in an *Al*Mg alloy does not produce the strong distortion of the s PDOS that is observed to occur in pure Mg. The reduction in the intensity of the s PDOS peak in the Mg KL_1V profile begins with the addition of a small amount of Al and becomes more marked as the Al concentration is increased (Fig. 2). The reduction in the distortion of the s PDOS by the core hole explains why the Mg KL_1V and $KL_{2,3}V$ Auger transitions approach the same profile as the Mg concentration is reduced in Al-Mg alloys (Fig. 4). It also explains the conclusion from Fig. 5(b) that the energy spread of the s PDOS around a core-ionized Mg site in an Al environment, as revealed by the Mg KL_1V spectrum of $\mathrm{Al_{85}Mg_{15}}$, does not match the energy spread of the s PDOS around an Al site in pure Al as revealed by the Al KV spectrum. Before attempting to explain the anomalous behavior of the s PDOS around a core-ionized Mg atom in Al-Mg alloys we first consider the conclusions that can be made about the band structure of Al-Mg alloys from x-ray spectra.

The final-state rule[2,7,15,16] says that the PDOS revealed by x-ray spectra will be the PDOS around neutral sites. The soft-x-ray spectra of Al-Mg alloys and their implications for the band structure of the alloys are not fully understood and have been the subject of some controversy which has been reviewed by Neddermeyer.[20] Perhaps the simplest model for the band structure of the Al-Mg alloys is where they form arrangements of $\mathrm{Al^{3+}}$ and $\mathrm{Mg^{2+}}$ ions and have a common band of conduction electrons with a bandwidth which varies smoothly with alloy composition between the 7- and 11.5-eV extremes of pure Mg and pure Al. The Al and Mg KV spectra of Al-Mg alloys, which reflect the local p PDOS around each site, are consistent with this interpretation: For a given alloy the spectra have a common bandwidth and almost identical profiles. On the other hand, the Al and Mg $L_{2,3}V$ x-ray spectra of Al-Mg alloys have different profiles. These transitions reflect the local s PDOS around each site though they also show additional structure at E_F caused by many-body processes. It was originally thought that the Al and Mg $L_{2,3}V$ x-ray spectra of Al-Mg alloys showed that each component had a separate band structure and that the bands had different widths.[21] However, a careful examination of the spectra by Neddermeyer[20] showed that the $L_{2,3}V$ spectra of each component could be interpreted as being consistent with a common bandwidth though it was not clear why the s PDOS had a different shape around Mg and Al sites.

In Fig. 6 we compare the changes induced in the soft-x-ray spectra of pure Mg and pure Al by forming dilute alloys. The spectra of the pure elements are shown by the full lines and those of the dilute alloys by the dashed lines. It is clear that the changes in the x-ray spectra of each element which result from forming a dilute alloy in the other constituent are opposite for the s and p PDOS. For the p PDOS the Al KV spectra show that the width of the p PDOS around an Al site is narrowed on alloying with Mg while the Mg KV spectra show that the p PDOS around a Mg site is broadened by the addition of Al. These changes in the p PDOS are to be expected from the common-band model in which the bandwidth depends on the alloy concentration. The changes induced in the shape of the s PDOS by alloying, as revealed by the $L_{2,3}V$ x-ray spectral profiles, are more complicated. The spectra show that alloying introduces different changes in the local s PDOS around Mg and Al sites, particularly at the bottom of the band. Thus the s PDOS at the bottom of the band around a Mg site falls on alloying while the s PDOS at

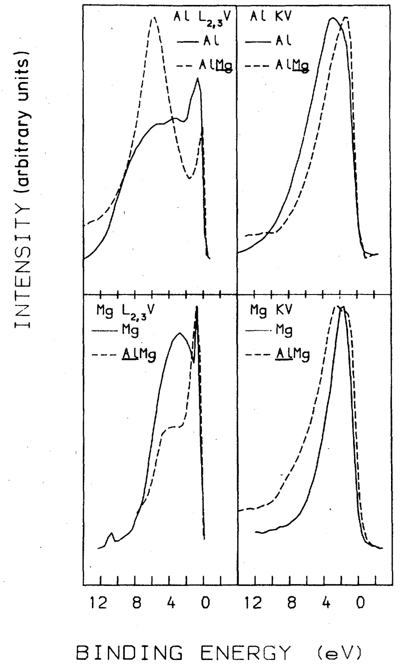

FIG. 6. This shows a comparison of the $L_{2,3}V$ and KV x-ray profiles of pure Al and pure Mg with those of dilute alloys. The x-ray spectra of the pure elements are shown by the full lines and those of the dulute alloys by the dashed lines. The spectra are from the compilation of Neddermeyer.[20] The underline denotes the majority constituent.

the bottom of the band around an Al site rises on alloying. We suggest that the explanation for these differences in the *s* PDOS around Al and Mg sites in the alloys is the different valence of the Al and Mg ions.[22–24] Theoretical work[2,4,6,7] has shown that in pure simple metals, core holes are screened by a distortion of the *s* PDOS so as to create a peak at the bottom of the band. The bandwidth is not increased by the core hole and the shape of the *p* PDOS is almost unchanged. By the equivalent-cores model we would expect a similar distortion of the *s* PDOS around an isolated Al^{3+} ion in Mg and we suggest that the $L_{2,3}V$ x-ray profile of Al in Al*Mg* reflects this behavior (Fig. 6). The calculations of von Barth and Grossmann[2,7] indicate that a valence or core-charge difference of $\Delta Z=+1$ between impurity and host does not strongly distort the *p* PDOS, which explains why the Al KV spectra of Al-Mg alloys reflect the width of the common band. When Mg is diluted in Al, however, the potential at an isolated Mg^{2+} site is reduced from that at a host site, i.e., $\Delta Z=-1$. This should lead to a fall in the local *s* PDOS at the bottom of the band and the Mg $L_{2,3}V$ x-ray profile of *Al*Mg (Fig. 6) shows that this is what happens. In *Al*Mg the shape of the *p* PDOS will be less affected than the *s* PDOS by the change in potential between the impurity and host sites and the Mg KV spectra will again just reflect the change in the width of the band induced by alloying.

This interpretation of the changes in the x-ray profile on alloying can be simply extended to explain the KLV Auger profiles (Fig. 4) since, by the final-state rule, these will reflect the *s* and *p* PDOS around core-ionized sites. The separation of the *s* and *p* PDOS peaks around a core-ionized Mg site in pure Mg results from the greater sensitivity of the former to the difference in core charge ΔZ between the core-ionized Mg and the host site. We expect this separation to be reduced as Al is added to Mg since the effect of this addition is to decrease the ΔZ between a core-ionized Mg and the average host site. The bandwidth of pure Al is larger than that of Mg and it is reasonable that in *Al*Mg alloys the Mg $L_{2,3}V$ x-ray and KL_1V Auger profiles show the *s* PDOS around neutral, and even core-ionized Mg sites to be more delocalized than in pure Mg. For the opposite situation of dilute Al in Mg we expect that even the *s* PDOS around a "neutral" Al site will show a distortion at the bottom of the band—indeed, this is how the Al^{3+} ion is screened. The presence of a core hole on the Al site should further distort the *s* PDOS which explains why in $\mathrm{Al}_8\mathrm{Mg}_{92}$ (Fig. 4) the Al KL_1V spectrum has more intensity at the bottom of the band than does the Al $KL_{2,3}V$ spectrum.

The calculations of von Barth and Grossman's[2,7] indicate that there is almost no change in the *p* PDOS around a site which differs from a host site by $\Delta Z=+1$ and this is borne out by Fig. 5(c). However, the *p* PDOS would not be expected to be completely insensitive to ΔZ and Fig. 5(c) shows that there is some shift of the *p* PDOS to the bottom of the band for $\Delta Z=+2$. For sufficiently large ΔZ even the formation of bound *s* states would not sufficiently screen the site and we might expect further distortions towards the bottom of the band in the *p* PDOS.

CONCLUSIONS

We have shown that the presence of a core hole on a Mg site in *Al*Mg alloys does not lead to a distortion of the local *s* PDOS. A consequence of this is that the Mg KL_1V and $KL_{2,3}V$ Auger transitions of such alloys have almost identical spectral profiles. The presence of a core hole on an Al site in Al*Mg* alloys does lead to a distortion of the local *s* PDOS, and the Al KL_1V and $KL_{2,3}V$ Auger transitions of such alloys show similar differences in spectral profile to those observed for pure simple metals. This behavior can be reconciled with the model of a common band for the alloys and with the observed x-ray spectral profiles, provided the difference in the valence of the constituents and in the bandwidths of the pure elements is taken into account. The addition of Al to Mg causes a widening of the common band and in the ground states of the alloys the increased potential on Al sites compared to Mg sites is screened by a local distortion of the *s* PDOS around Al sites. The *p* PDOS around each type of site is changed little by alloying. The difference in potential between a core-ionized Mg site and an average site in an *Al*Mg alloy is small and there is no need for a distortion of the local *s* PDOS in order to screen the core hole. A core-ionized Al site in an *Al*Mg alloy will have a significantly increased potential, $\Delta Z=+2$ over an average site and the local *s* PDOS will be distorted to screen the site. Figure 5(c) shows that a $\Delta Z=+2$ difference between the local site and a host site causes some distortion of the local *p* PDOS.

Although the changes induced in the Mg and Al KLV profiles by alloying can be readily accounted for in terms of the charge difference ΔZ between the core-ionized site and an average lattice site, it is harder to account for the convergence of the Mg KL_1V and $KL_{2,3}V$ Auger profiles in Mg-Zn alloys[9] since in this system both constituents have nominally the same valence. The free-electron bandwidth of Zn, calculated from the electron density, though smaller than that of Al, is still wider than that of Mg and it may be that the compression of the Mg charge density in Mg-Zn alloys compared to pure Mg is in some way responsible for the difference in core-hole screening in the two systems.

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