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## The orbital character of the core-hole screening charge in metallic Mg

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**Abstract.** Atomic-like transition rate calculations have been performed for the  $KL_1V$  and  $KL_{2,3}V$  Auger processes in metallic magnesium. The valence screening configuration is varied in order to reproduce the experimental  $KL_1V_i:KL_1V_p$ ,  $KL_{2,3}V_i:KL_{2,3}V_p$ , and  $KL_1V:KL_{2,3}V$  intensity ratios. The theoretical results are in best agreement with experiment for a screening configuration surrounding the  $1s$  core-hole of  $3s^13p^2$ . This result is in conflict with previous analyses of core-hole screening in magnesium.

### 1. Introduction

The simple metals have been the subject of much experimental and theoretical attention. X-ray [1–4] and ultraviolet [4–6] photoemission, Auger electron spectroscopy [7–13] and soft x-ray absorption and emission spectroscopies [10, 14, 15] have been used to measure the densities of states, core level binding energies and the changes in the  $s$  and  $p$  components of the density of states arising from the presence of one or more core-holes. On the theoretical side, it is now recognised that the calculation of local densities of states must take account of the presence of core-holes and initial attempts to calculate Auger and x-ray lineshapes based upon ground state densities of states [16, 17] have been superseded by improved one-electron models [18–21] which take account of the core-hole structure. The theoretical position is summarised by the final state rule [19–26] which dictates that the shapes of the  $s$  and  $p$  valence contributions to x-ray and Auger profiles are given by the local electronic structures in the final states whereas the intensities are determined by the valence configurations in the initial states. Recently theoretical studies have been extended to include Mahan–Nozières–DeDominicis (MND) [27, 28] type calculations incorporating many body effects.

An interesting consequence of comparing calculated and experimental Auger profiles is that the results can reveal information on the local valence charge screening core-hole states. This subject has recently been reviewed [26, 29]. It is clear from both Auger and x-ray studies that the screening response of the valence electrons of a simple metal to the presence of a core-hole involves the creation of a peak at the bottom of the  $s$  DOS. The core-hole does not change the *shape*, though it may change the intensity, of the  $p$  DOS around a core-ionised site. These conclusions when combined with the final state rule and a consideration of matrix elements effects make it possible to understand the

shape of the KLV Auger profiles of Na, Mg, and Al [10, 20, 26] and to interpret the changes that take place in the KLV spectra of AlMg alloys [30]. They also give insight into the understanding of the more complex spectra of alloys between simple metals and d band metals [31, 32].

In this work, we show how the comparison of the experimental profiles of the Mg  $KL_1V$  and  $KL_{2,3}V$  transitions with the results of atomic-like transition rate calculations can be used to deduce the core-hole screening configuration around a 1s core-hole in Mg metal. Our approach is to compare the experimental results for the total  $KL_1V : KL_{2,3}V$  intensity ratio and the valence s and p contributions to the partial intensity ratios,  $KL_1V_s : KL_1V_p$  and  $KL_{2,3}V_s : KL_{2,3}V_p$  with computations of the dependence of these ratios on possible screening configurations.

## 2. Experimental details

The experimental KLV Auger spectrum of Mg is shown in figure 1. It was measured using Al  $K\alpha$  excitation of a polycrystalline magnesium sample, mechanically scraped for cleanliness, and recorded using an AEI ES200 electron spectrometer equipped with a multidetector system [33]. The experimental procedure is described in reference [4]. The spectrum of figure 1 is in good agreement with the results of other workers [34]. The main features of the spectrum shown in figure 1 are, in decreasing kinetic energy; the  $KL_{2,3}V$  transition, three accompanying plasmon energy loss satellites, the double peaked  $KL_1V$  transition with an accompanying plasmon loss satellite and two weak, sharp features, arising from the C 1s impurity photoemission line and a plasmon gain satellite on the strong  $KL_{23}L_{23} : ^1D_2$  Auger line. The tail of this latter feature appears on the extreme low kinetic energy region of the spectrum. The extreme high energy region of figure 1 shows the  $KL_{2,3-L_{2,3}}L_{2,3}V$  Auger vacancy satellite transitions [35].

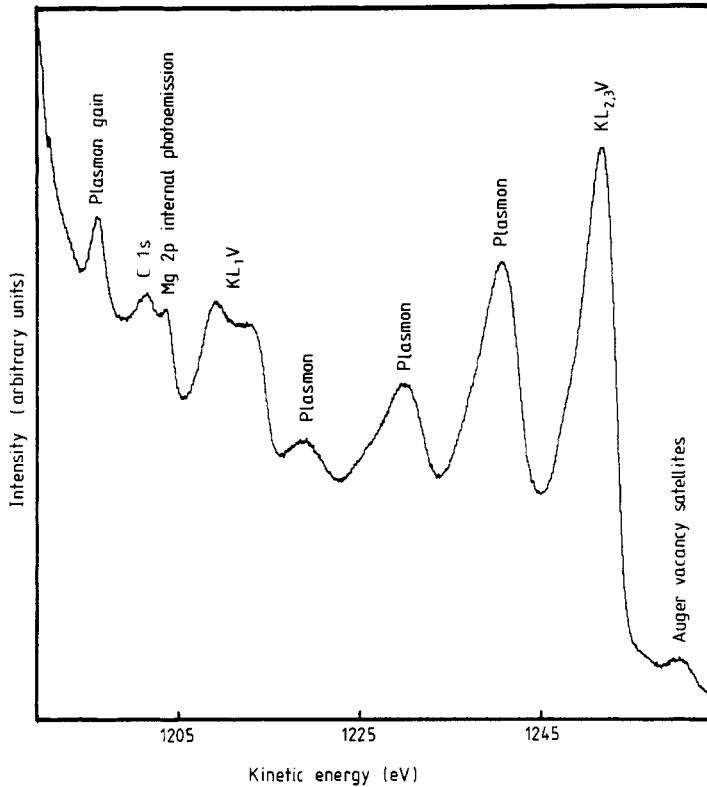
The two clearly identifiable peaks in the  $KL_1V$  profile belong to  $KL_1V_s$  and  $KL_1V_p$  transitions. Any reasonable attempt to deconvolute the  $KL_1V$  profile into these overlapping components yields an intensity ratio  $KL_1V_s : KL_1V_p$  of  $\sim 1 : 1$ . It is more difficult to establish the relative strength of the corresponding features in the  $KL_{2,3}V$  profile since matrix element effects diminish the relative importance of the  $KL_{2,3}V_s$  peak and it is not clearly resolved from the stronger  $KL_1V_p$  contribution. However this component can be observed as a shoulder on the low kinetic energy side of the  $KL_{2,3}V$  profile (figure 1) and by using the relative positions and shapes of the  $KL_1V_s$  and  $KL_1V_p$  components of the  $KL_1V$  profile as a guide one can reproduce the  $KL_{2,3}V$  profile with a  $KL_{2,3}V_s : KL_{2,3}V_p$  ratio of  $\sim 1 : 4$ .

The ratio of the total intensities,  $KL_1V : KL_{2,3}V$ , can be obtained by subtracting a crude background from the data of figure 1 and measuring the relative areas. To an accuracy of about 10% this gives a  $KL_1V : KL_{2,3}V$  intensity ratio of 0.41 : 1. A similar result, 0.37 : 1 is obtained from van Attekum and Trooster's work [34] in which they systematically subtract the plasmon loss contributions to the spectrum.

These experimental results for the relative intensity of components of the KLV Auger spectrum of metallic Mg are shown in table 1. The errors quoted are what we consider to be upper estimates of the uncertainty in the results.

## 3. Theory and results

Ideally the calculation of Auger transition rates involves the evaluation of matrix elements in which the radial wavefunctions are obtained from separate self consistent



**Figure 1.** The region of the KLV Auger spectrum of metallic Mg. At the extreme high kinetic energy end of the spectrum there is a weak feature caused by Auger vacancy satellite processes [33]. To low energy of this is the intense  $KL_{2,3}V$  transition with three accompanying plasmon loss peaks to lower energy. The two component  $KL_1V$  transition occurs to low energy of the plasmons. To low energy of the  $KL_1V$  transition there are three peaks which, in order of decreasing energy, are the Mg 2p internal photoemission line, a small C 1s impurity line, and a plasmon gain satellite from the  $KL_{2,3}L_{2,3};^1D$  line. The kinetic energy scale is referenced to the vacuum level.

**Table 1.** Transition rates in units of  $10^{-4}$  per atomic unit of time.

Initial state valence configuration	$KL_1V_s$ / $KL_1V_p$		$KL_1V_s$ / $KL_1V_p$	$KL_{2,3}V_s$ / $KL_{2,3}V_p$		$KL_{2,3}V_s$ / $KL_{2,3}V_p$	$KL_1V$ / $KL_{2,3}V$
	$KL_1V_s$	$KL_1V_p$	$KL_1V_s$ / $KL_1V_p$	$KL_{2,3}V_s$	$KL_{2,3}V_p$	$KL_{2,3}V_s$ / $KL_{2,3}V_p$	$KL_1V$ / $KL_{2,3}V$
$3s^23p^0$	1.65	—	—	2.60	—	—	0.80
$3s^13p^1$	0.82	0.38	2.14	1.30	1.56	0.84	0.42
$3s^23p^1$	1.65	0.38	4.28	2.60	1.56	1.67	0.49
$3s^13p^2$	2.47	2.31	1.07	3.91	9.33	0.42	0.36
$3s^23p^2$	4.94	2.31	2.14	7.81	9.33	0.84	0.42
Experiment	—	—	$1.0 \pm 0.2$	—	—	$0.3 \pm 0.1$	$0.4 \pm 0.1$

field treatments of the local electronic structure in the initial and final states. Such calculations are complicated by contributions arising from the non-orthogonality of spectator orbitals in the initial and final states and have only been attempted for a few cases. Usually Auger matrix elements are evaluated within the frozen orbital approximation in which the radial wavefunctions of the initial and final states correspond to the same potential. This has the advantage of avoiding non-orthogonality effects and allows the expressions for the transition rates to be written as combinations of angular terms and radial matrix elements which involve only those orbitals participating in the transition. Due to the large changes in atomic wavefunctions caused by the presence of a core hole the majority of Auger transition rate calculations employ atomic and continuum wave functions evaluated for the core-ionised potential of the initial state. McGuire [36–38] has produced extensive tabulations of atomic Auger radial matrix elements evaluated in this way using wavefunctions obtained from Hermann and Skillman's treatment of atomic structure calculations [39]. For transitions involving only core levels and excepting Coster–Kronig transitions and transitions strongly influenced by relativistic effects, the results of McGuire's atomic calculations are usually in good agreement with experimental results for solids [25], a finding which can be attributed to the expectation that the wavefunctions of atomic core electrons are almost independent of phase.

For Auger transitions involving valence levels there are a number of problems in attempting to extend an atomic analysis to the solid state not least of which is deciding which is the appropriate valence configuration in the solid. It is this problem, in the particular context of the metallic state of Mg, which is addressed in this work. We begin with the final state rule which indicates that for an Auger transition involving the Mg valence levels the intensity of valence s and p contributions is given by the local electronic structure in the initial, core-ionised, state. Since the results of XPS experiments show that core-hole states in metals are long lived the initial state should be considered to be a screened core-ionised site. Consequently we expect to be able to probe the character of the screening charge by comparing the contributions of s and p valence electrons to relative Auger intensities. In this work we consider the core–core–valence (CCV) transitions and for these processes the valence wavefunctions in both the initial and final state correspond to a core-ionised site. We argue that McGuire's matrix elements, which are evaluated in accordance with the frozen orbital approximation and use wavefunctions appropriate to a core-ionised potential, should be quite a good description of CCV processes in a simple metal. In support of this view we note that: (i) the Auger matrix elements include the localised wavefunctions of core-hole states and this ensures that the only parts of the radial wavefunctions of valence orbitals that contribute to Auger transition rates are those in the core region, (ii) the requirement that valence wavefunctions be orthogonal to core wavefunctions probably means that the core region of the valence wavefunctions is not strongly perturbed by the solid state environment, and (iii) the presence of the core-hole in the initial state will deepen the potential on the site and draw in the valence wavefunctions weakening the influence of the solid state environment. However justified we are in using atomic calculations to probe valence configurations in a metal it is clear that our approach will only succeed if the results of the transition rate calculations show a strong dependence on the assumed form of the valence configuration. We show later that in the calculations presented here this is indeed the case.

In order to calculate KLV Auger transition rates for Mg with different occupations of valence s and p configurations it is necessary to evaluate expressions corresponding

to atoms with several open subshells. Fortunately McGuire [38] has given general expressions for Auger transition rates for systems with several unfilled subshells and these have recently been simplified for several particular cases by Cubiotti, Laine and Weightman [40]. In this work we have used McGuire's formalism and atomic matrix elements to calculate the  $KL_1V$  and  $KL_{2,3}V$  transitions of magnesium atoms with valence configurations  $3s^23p^0$ ,  $3s^13p^1$ ,  $3s^23p^1$ ,  $3s^13p^2$ , and  $3s^23p^2$ .

In our calculations of the transition rate for  $KL_1V_p$  and  $KL_{2,3}V_p$  transitions for Mg we require matrix elements involving the  $3p$  orbital which is not normally occupied in the free atom. In a preliminary treatment [41], restricted to  $KL_1V$  transitions, we combined McGuire's [36, 37] matrix elements for Mg  $KL_1V_s$  processes with his matrix elements for Al  $KL_1V_p$  processes. In this work we have followed the same in procedure in calculating  $KL_{2,3}V$  transition rates. We have also calculated transition rates for both  $KL_1V$  and  $KL_{2,3}V$  transitions using only Al matrix elements. The results obtained using only Al matrix elements are shown in table 1.

A comparison of results obtained for the  $KL_1V_s$  [41] and  $KL_{2,3}V_s$  transitions using Mg and Al matrix elements shows that this difference introduces changes of about 25% in the absolute values obtained for these transition rates. Excepting the  $3s^23p^0$  configuration the use of Mg matrix elements for transitions involving  $3s$  orbitals reduces the results for the  $KL_1V_s:KL_1V_p$ ,  $KL_{2,3}V_s:KL_{2,3}V_p$  and  $KL_1V:KL_{2,3}V$  ratios shown in table 1 by  $\approx 23\%$ ,  $14\%$  and  $10\%$  respectively. In contrast to this relatively small dependence of our results for the intensity ratios on atomic number we find a much stronger dependence of the results for the  $KL_1V_s:KL_1V_p$  and  $KL_{2,3}V_s:KL_{2,3}V_p$  intensity ratios on the assumed valence configuration (table 1). These ratios vary by at least a factor of two and up to a factor of four with changes in the valence configuration (table 1). That our results depend so much more strongly on the assumed form of the valence configuration than on atomic number supports the idea that Auger intensity ratios will be influenced more by changes in the valence configuration in the solid than by changes in the radial wavefunctions of the valence electrons in the solid state environment.

Before analysing our results we note an important respect in which our calculations differ from purely atomic calculations. In an atomic calculation one evaluates the transition rate from the ground term of the initial configuration to all the terms of the final state configuration. In the calculations presented here we have assumed that the screening charge attracted to the core-ionised initial state is able to populate all the terms of the initial screening configuration so the calculated rates include contributions from transitions between all the terms of the initial configuration to all the terms of the final configuration. This is a reasonable assumption since the Slater integrals [42] giving rise to the term splittings are either small ( $G^0(1s, 3s)$  and  $G^1(1s, 3p) \approx 0.28$  eV) or comparable ( $G^1(3s, 3p) \approx 4.8$  eV) to the extra-atomic relaxation energy (4.8 eV [2, 25]) accompanying the creation of a core-hole in Mg metal. It is the contribution from the large number of terms present in the  $3s^13p^2$  and  $3s^23p^2$  initial-state valence configurations which explains the large transition rates obtained for these configurations (table 1). However it is important to note that even if we drop the assumption that the screening charge is able to populate all the terms of the initial states and restrict the calculation to transitions from the ground term of each configuration this gives a uniform reduction in all the transition rates and leaves the relative rates, upon which our analysis is based, unchanged.

The results in table 1 show that, except for the free atom case,  $3s^23p^0$ , the ratio of the total intensities of the  $KL_1V$  and  $KL_{2,3}V$  transitions does not depend strongly on the assumed form of the valence configuration in the initial state and that to within the

experimental uncertainty all the results obtained for this ratio can be considered to be in good agreement with experiment. The fact that the  $3s^23p^0$  configuration gives a result for this ratio which is outside of the experimental uncertainty confirms the expectation that there is some admixture of  $3p$  states into the valence configuration in Mg metal.

The results for the  $KL_1V_s:KL_1V_p$ ,  $KL_{2,3}V_s:KL_{2,3}V_p$  intensity ratios, which depend very strongly on the assumed form of the valence configuration (table 1), show that only the  $3s^13p^2$  configuration gives ratios in agreement with the experimental results. The result obtained for the most accurately determined ratio,  $KL_1V_s:KL_1V_p$ , is excellent and that obtained for the  $KL_{2,3}V_s:KL_{2,3}V_p$  ratio is within the experimental uncertainty. All the other configurations considered in table 1 yield results that are quite incompatible with experiment for both these ratios; they predict  $KL_1V$  profiles dominated by  $KL_1V_s$  peaks and  $KL_{2,3}V$  spectra in which the  $KL_{2,3}V_s$  components are clearly resolved. The same conclusions are reached if the calculations are performed using a combination of Mg matrix elements for transitions involving the  $3s$  orbital and Al matrix elements for transitions involving the  $3p$  orbital [41].

#### 4. Discussion

Band structure calculations [4, 43] indicate that the local configuration in the ground state of metallic Mg has roughly equal  $3s$  and  $3p$  character suggesting a local configuration  $3s^13p^1$ . The creation of a core-hole is expected to attract screening charge to the site in the metal. Perfect local screening implies the addition of a single electron to the local configuration, the extreme cases of  $s$  and  $p$  screening giving configurations of  $3s^23p^1$  and  $3s^13p^2$  respectively. The unlikely possibility of a single core-hole being screened by two valence electrons can be represented by  $3s^23p^2$ .

It is clear from our results that the only configuration which gives agreement with the experimental KLV Auger intensity ratios of Mg is  $3s^13p^2$  and that this configuration is far superior in this respect to the others and in particular to  $3s^23p^1$ . In terms of the final state rule and simple model of the local electronic structure of metallic Mg advanced above, the core-hole is screened by valence charge of  $p$  character.

Our conclusion that core-holes in metallic Mg are screened by valence charge of  $p$  character conflicts with the results of other studies which suggest that in  $sp$  band systems core-hole screening is affected by  $s$  valence charge. Thus core-holes in Li [18], Be [19] and Na [20] are all thought to be screened by valence charge of  $s$  character. Our results also contradict directly two other studies [11, 44] which suggest that core-holes are screened by  $s$  valence charge in metallic Mg; Jennison and co-workers [44] reached this conclusion from considerations of the energies of singly and doubly ionised core states in Mg, while Davies and co-workers [11] came to the same conclusion from an analysis of the lineshapes of CVV processes in Mg. We should note that there is no disagreement with the view that the presence of a core-hole in Mg leads to a distortion of the local  $s$  density of states with the creation of a peak at the bottom of the band and that the *shape* of the  $p$  density of states is much less affected by the presence of the core-hole. To this extent a large contribution to the screening of the core-hole is achieved by the distortion of the local  $s$  density of states. The question we are concerned with here is not the *shape* of the local density of states occupied by the screening charge but its magnitude and orbital character.

By calculating the binding energies of singly and doubly ionised core-states in Mg from a  $\Delta$ SCF Hartree–Fock procedure in which the local valence configuration was

varied, Jennison and co-workers [44] concluded that the ground state, singly core-ionised and doubly core-ionised states in Mg metal are best described by local valence configurations  $3s^13p^1$ ,  $3s^23p^1$ , and  $3s^23p^2$  respectively. Jennison and co-workers' [44] work could be criticised on the grounds that it did not allow for effects due to the compression of the valence wavefunctions in the metal. Since the radial dependence of the 3s and 3p wavefunctions of Mg are similar, however, it is unlikely that compression of the valence charge would produce a sufficient change in the *relative* 3s and 3p contribution to the total energy that a different 3s to 3p occupancy ratio would be predicted by the  $\Delta$ SCF calculations. A possible explanation of the discrepancy between our conclusions and the  $\Delta$ SCF study is that the latter, since it is a study of the energetics of core-ionised states is significantly less sensitive to the valence wavefunctions than is the present study which is concerned with the relative intensity of spectral components the transition rates for which involve the valence orbitals directly.

It is also difficult to resolve the discrepancy between our conclusions and the results of Davies and co-workers' [11] study of the lineshapes of KVV and  $L_{2,3}$ VV transitions observed from Mg metal. Davies and co-workers [11] noted that although these two processes create identical final states their matrix elements show a different dependence on the angular momentum character of the valence orbitals. By comparing the spectral profiles of the two transitions with combinations of convolutions of the final ss, sp and pp densities of states weighted by the appropriate transition rates Davies and co-workers [11] were able to confirm the validity of the final state rule and determine the relative strength of valence s and p screening charge around a core-ionised site. If the local density of states in Mg metal is approximately  $3s^13p^1$  Davies and co-workers' [11] result suggest that core-holes are screened by valence charge of s character in direct contradiction to the results reported here. The solution to this contradiction may lie in some observations of Almladh and Morales [27, 28].

Recently Almladh and Morales [27, 28] have calculated the CVV Auger profiles of a number of simple metals, including Mg, in a MND framework, in which the valence electrons are represented by different one electron Hamiltonians in the initial and final states. Their calculations indicate that in Mg the local valence configuration in the ground state is  $3s^{0.88}3p^{0.94}$  and that in the presence of a core-hole this changes to  $3s^{1.29}3p^{1.56}$ . Their result that the additional screening electron attracted to the core-ionised site occupies valence states of predominantly p character is in keeping with the results of the work reported here. In seeking to explain the discrepancy between their conclusion of predominantly p state screening with Davies and co-workers' [11] result Almladh and Morales draw attention to differences in the treatment of the final state Auger orbitals in the two studies. Almladh and Morales [27, 28] argue that Davies and co-workers' [11] derivation of the continuum wavefunction used in calculating transition rates leads to an overestimate of the amplitudes of higher l components and to a corresponding underestimate of the amount of screening charge in p orbitals. If this view is correct then it might be possible to reconcile Davies and co-workers' [11] results with the conclusions of Almladh and Morales [27, 28] and this work that core-ionised sites in Mg are screened by charge of predominantly p character.

## 5. Conclusions

We have calculated the  $KL_1V_s:KL_1V_p$ ,  $KL_{2,3}V_s:KL_{2,3}V_p$  and  $KL_1V:KL_{2,3}V$  Auger intensity ratios of Mg within an atomic framework and as a function of the local valence



configuration. The results of the calculations depend strongly on the assumed form of the valence configuration and show clearly that only an assumption of p state screening of core-holes, corresponding to a local configuration of  $3s^13p^2$ , is consistent with the experimental values for the Auger intensity ratios. The assumption of s state screening, with a  $3s^23p^1$  local configuration, yields results quite incompatible with experiment.

The conclusion of p state screening of core-holes in Mg is in agreement with recent MND calculations [27, 28] but conflicts with earlier studies of the energetics of core-hole states in Mg [44] and of the profiles of the KVV and  $L_{2,3}$ VV Auger transitions [11].

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