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Core-hole screening in metallic magnesium

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Abstract. An atomic-like formalism has been used to calculate the KL_1V Auger transition rate for magnesium as a function of the initial-state valence configuration. The transition rate for KL_1V processes involving valence s and p holes, KL_1V_s and KL_1V_p, have been calculated for several valence configurations. A comparison between the theoretical and the experimental values of the KL_1V_s:KL_1V_p ratio suggests that a 1s core hole in metallic magnesium is screened by a valence charge of p character.

The KL_1V Auger profile of solid magnesium consists of two peaks of similar intensity, the one at higher energy arising from valence p electrons, that at lower energy from valence s electrons. The s-like part of the profile in the presence of a core hole shows that the s density of states is very different from that of the ground state. The ratio of $KL_{2,3}V$ to KL_1V in the atom has been calculated previously [1]. We have extended the formalism [2] in order to apply it to the solid, and have calculated the relative intensities of the s and p contributions to the KL_1V spectrum individually. In performing these calculations, we must make a choice of screening configuration surrounding the 1s hole, and we have made the choices $3s^23p^0$, $3s^13p^1$, $3s^23p^1$, and $3s^13p^2$, which correspond to the atomic ground state, the metallic ground state, s-like screening and p-like screening. The calculated values and ratios are shown in table 1.

The principal point to notice from table 1 is that the $3s^13p^2$ initial-state screening configuration (p screening) is the only one that gives a realistic KL_1V_s:KL_1V_p intensity ratio, 0.83, and that the s screening configuration, which has previously been supposed

Table 1. Calculated KL_1V Auger transition rates for Mg as related to the core-hole screening configuration. (The rates are given in units of 10^{-4}/all of time.)

Initial-state valence configuration	KL_1V_s	KL_1V_p	KL_1V_s/KL_1V_p
$3s^23p^0$	1.27	—	—
$3s^13p^1$	0.64	0.38	1.64
$3s^23p^1$	1.27	0.38	3.34
$3s^13p^2$	1.91	2.31	0.83

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to be correct [3], yields the ratio furthest removed from the experimental value. From this, we conclude that a 1s core hole in magnesium is predominantly screened by a valence charge of p character.

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