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How are changes in Auger parameter related to charge transfer in binary systems?

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Abstract. Shifts in the modified Auger parameter of atoms in binary compounds provide a pair of parameters diagnostic of an electronic relaxation mechanism.

The modified Auger parameter α' [1] has become established as a convenient measure of the efficiency of an atom in screening localised core holes in different environments. The approach of Thomas [2] provides a simple theoretical framework for interpreting $\Delta\alpha'$, the shift in Auger parameter of an atom relative to its value in the elemental solid. Then

$$\Delta\alpha' = (\mathrm{d}k/\mathrm{d}N)_q + (k - 2\,\mathrm{d}k/\mathrm{d}N)\Delta(\mathrm{d}q/\mathrm{d}N) + \Delta(\mathrm{d}U/\mathrm{d}N) \qquad (1)$$

where q is the *initial-state* charge on the atom in the solid, k is the change in core potential when a valence electron is removed, N is the core occupation number, and $\mathrm{d}U/\mathrm{d}N$ the rate of change of environmental potential with N. The first term gives the dependence of intra-atomic screening on q, the second the efficiency of relaxation by charge transfer in response to the core hole, and the third the effect of environmental screening.

In the case of 'perfect' charge transfer in both elemental solid and binary compounds (exactly one charge transferred to the atomic site per core hole), the second and third terms do not vary with environment, and $\Delta\alpha' = (\mathrm{d}k/\mathrm{d}N)_q$, so there is a direct relationship between $\Delta\alpha'$ and the initial-state charge. In a binary system $\Delta\alpha'$ would then be opposite in sign for the two atomic species.

Using a Jost cavity model Waddington and co-workers [3] have shown that there is $(1 - 1/\varepsilon)$ of a screening charge per core hole transferred to the atomic site to first order (ε is the effective permittivity of the medium). This implies that $\Delta(\mathrm{d}q/\mathrm{d}N)$ in equation (1) is $\Delta(-1/\varepsilon)$. Typically $\mathrm{d}k/\mathrm{d}N \simeq 2$ eV and $k \simeq 10$ eV so for $\varepsilon \geqslant 10$ (the usual range for semiconductors) the environmental dependence of the charge-transfer relaxation is substantial; furthermore, it will be of the *same sign* for both atomic components.

Surprisingly there are relatively few binary systems AB where $\Delta\alpha'$ is available for both components—a selection is given in table 1. In no case are both Δ'_A and Δ'_B above zero (better screening for both atoms). AgZn and AgMg have Δ'_A and Δ'_B opposite in sign indicating that differences in intra-atomic screening characteristic of the initial-state charge dominate [4]. Semiconductors are usually characterised by $\Delta\alpha'_A$ and $\Delta\alpha'_B$ both being below 0, consistent with imperfect charge-transfer screening as well as

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Table 1. Dual modified Auger parameter shifts in binary compounds.

Compound	Reference	A	$\Delta\alpha'_A$ (eV)	B	$\Delta\alpha'_B$ (eV)
AuMg	[4]	Au	+0.14	Mg	−0.65
AuZn	[4]	Au	+0.22	Zn	−0.32
$MoSi_2$	[4]	Mo	−0.1	Si	+0.7
Na_3Sb	[1, 5]	Na	−1.1	Sb	−1.7
Cs_3Sb	[1, 5]	Cs	−1.0	Sb	−0.7
CdTe	[1, 5]	Cd	−1.2	Te	−1.4
PbTe	[3]	Pb	−0.55	Te	−0.8
GaAs	[1, 5]	Ga	−1.2	As	−0.8
GaP	[1, 5]	Ga	−1.3	P	+0.6

initial-state charge effects. Better models are needed to separate intra-atomic and extra-atomic components; in particular one needs to go beyond the specification of the screening environment by a single parameter ε.

Building up a comprehensive pattern of *dual* Auger parameter shifts for a wide range of binary compounds will enhance our understanding of electronic relaxation in solids.

References

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[5] Wagner C D 1983 *Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy* ed. D Briggs and M Seah (London: Wiley) Appendix 4