# Abstract: One-electron theory of Auger lineshapes: Silicon $L_{23}VV$ and $L_1L_{23}V$

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For Auger spectroscopy to be an effective local probe of surface bonding as well as constitution, we must have a theory of Auger lineshapes which relates the latter to the chemical environment of the target atom. Previous theoretical work by Feibelman, McGuire, and Pandey on silicon[1,2] failed to reproduce the experimentally observed $L_{23}VV$ or $L_1L_{23}V$ lineshapes, despite the inclusion of surface, matrix elements, and attenuation effects. The present paper shows that Feibelman *et al.* used a Bloch function normalization inconsistent with the atomic orbital basis used to calculate the matrix elements, and that this normalization, when included in their simplified version of the theory (where surface effects, nondiagonal local density matrices, and small matrix elements are neglected) yields excellent agreement between the theoretical and experimental $L_{23}VV$ line. The normalization effect causes a dramatic decrease in the *ss* and *sp* compared to *pp* final hole states and is the probable explanation for the *pp* dominance observed in Li and Al as well as Si. However, this correction does not yield an acceptable $L_1L_{23}V$ lineshape. McGuire[3] has noted a similar problem in atomic argon and these results suggest that where correlation effects are important in atomic Auger spectroscopy, the effects persist in the solid state.

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[1]P. J. Feibelman, E. J. McGuire, and K. C. Pandey, Phys. Rev. **15**, 2202 (1977). This paper reports incorrect results which are corrected in Ref. 2.

[2]P. J. Feibelman and E. J. McGuire, *Valence Band Auger Lineshapes for Si Surfaces: Simplified Theory and Corrected Numerical Results* (to be published).

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# Abstract: Solid state and atomic features in the valence-band Auger spectra of copper, silver, and gold

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Lander[1] has suggested that Auger spectra could yield information about the valence-band density of states of solids. For some free-electron-like elements, the Auger spectra have been shown to be related to the density of states while for other solids the spectra show features attributed to atomiclike final states. Sawatzky[2] has recently proposed a criterion for predicting bandlike or atomiclike features in Auger spectra and this criterion is examined here using high-resolution measurements of core–valence–valence Auger spectra for copper, silver, and gold. We find that features in the $L_3VV$ Auger spectrum for Cu are sharp and atomiclike, whereas those of the $M_{4,5}VV$ Auger transition in Ag are broader and those of the $M_{6,7}VV$ Auger transition in Au are still broader. The experimental data are compared with self-convolutions of the valence-band density of states with good correspondence obtained only for Au. Values of $U_{\text{eff}}$, the effective energy required to excite two holes on the same atom, are derived from the energies of the prominent features and found to be 7.7, 5.0, and 5.0 eV for Cu, Ag, and Au, respectively. These values of $U_{\text{eff}}$ are compared with values of twice the *d*-band width (6, 7, and 11 eV for Cu, Ag, and Au), as suggested by Sawatzky.[2] This comparison provides a useful means for distinguishing the atomic like Auger spectrum of Cu from the bandlike spectrum of Au. This work is described in more detail elsewhere.[3]

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[2]G. A. Sawatzky, Phys. Rev. Lett. **39**, 504 (1977).

[3]C. J. Powell, Solid State Commun. (in press).

  