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ANGLE-RESOLVED PHOTOEMISSION STUDIES OF Ag, Au, and Pt

R.F. Davis, K.A. Mills, G. Thornton, S.D. Kevan, and D.A. Shirley

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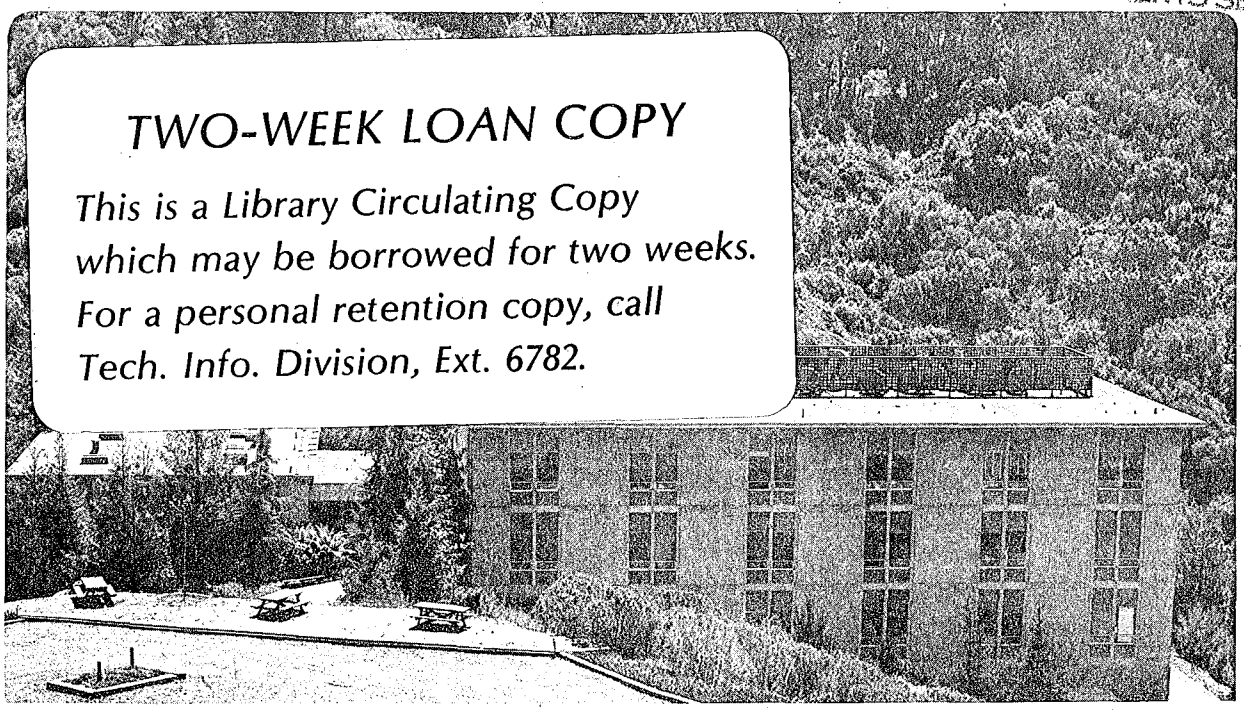

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ANGLE-RESOLVED PHOTOEMISSION STUDIES OF Ag, Au, AND Pt*

R.F. Davis, K.A. Mills, G. Thornton, S.D. Kevan, and D.A. Shirley

Materials and Molecular Research Division, Lawrence Berkeley Laboratory and Department of Chemistry, University of California, Berkeley, California 94720

An important question regarding the technique of angle-resolved photoemission (ARP) is the extent to which it can be used to determine experimental valence-band dispersion relations $E_i(\vec{k})$ for single crystalline solids. In the case of the 3d and 4d transition metals, studies of copper,[1,2] nickel,[3] palladium,[4] and silver,[5] show that a model based on the assumption of direct interband transitions (direct-transition model)[1] may be used, in conjunction with an appropriate final-state dispersion relation $E_f(\vec{k})$, to elucidate $E_i(\vec{k})$ for these materials along several high symmetry lines (primarily $\Gamma\Lambda L$) in k-space. To answer this question more generally, we have undertaken an extensive study of the valence band structures of other transition metals along various k-space lines. To date, studies have been extended to the (111) faces of the 5d metals Pt and Au along with the Pt(100) ((5 x 20) surface structure) face, and the (110) and (100) faces of Ag. The experiments were all conducted at SSRL, using synchrotron radiation in the range 6 eV $\leq h\nu \leq$ 34 eV. The results of these studies, combined with our previous Ag(111) work at these energies,[5] allow us to invoke important conclusions concerning the relationships between ARP data, $E_i(\vec{k})$ and $E_f(\vec{k})$ for these materials. Several are summarized below.

For each crystal face investigated, the direct-transition model, along with a simple quasi-free-electron $E_f(\vec{k})$, was sufficient to determine experimental $E_i(\vec{k})$ relations along the appropriate k-space line that were in general agreement with theoretical RAPW band structure calculations.[6-8] Essentially, we required $E_f(\vec{k})$ to be of the form $(\hbar^2/2m^*)|\vec{k} + \vec{G}|^2 + V_o$, where $\vec{G}$ is a reciprocal lattice vector, fitting this relation to the appropriate calculated bulk conduction band near the center of the line under investigation, with the inner potential V_o and the reduced mass m^* as free parameters. An additional shift of V_o was necessary for Ag(110) and Pt(100) data, to obtain better agreement with theoretical bands.

While generally excellent agreement between experimental and theoretical

bands was found for Ag, as was the case for other 3d and 4d metals,[1-4] substantial disagreement was observed for Pt and Au in parts of the Brillouin zone. This is probably an indication that further theoretical work is needed for these more complicated elements. The agreement in Ag is illustrated by Fig. 1, where experimental and theoretical[8] bands are compared for all three high-symmetry directions.

The determinations of $E_i(\vec{k})$ for the Λ directions were relatively simple because peaks in the ARP spectra of (111) faces were essentially all attributable to primary direct transition. However, the Σ, Σ', and Δ directions were complicated by secondary emission peaks[9] and dispersionless density-of-states (DOS) features in the spectra of the (100) and (110) faces. Peak intensity resonances associated with the bulk conduction band structure near Γ were observed for each crystal face, and these simplified the assignment of peaks in the ARP spectra. The relationship between these resonances, which appear to be rather general phenomena, and $E_f(\vec{k})$, will be discussed.

In summary, it is clear from these and other studies that the ARP technique, in conjunction with the direct-transition model, is generally applicable to valence band mapping in single crystals, provided that a suitable final-state dispersion relation can be calculated. However, complications like those observed in the ARP spectra of Ag, Pt, and Au may make the determination of $E_i(\vec{k})$ relations considerably more difficult for more complicated systems.

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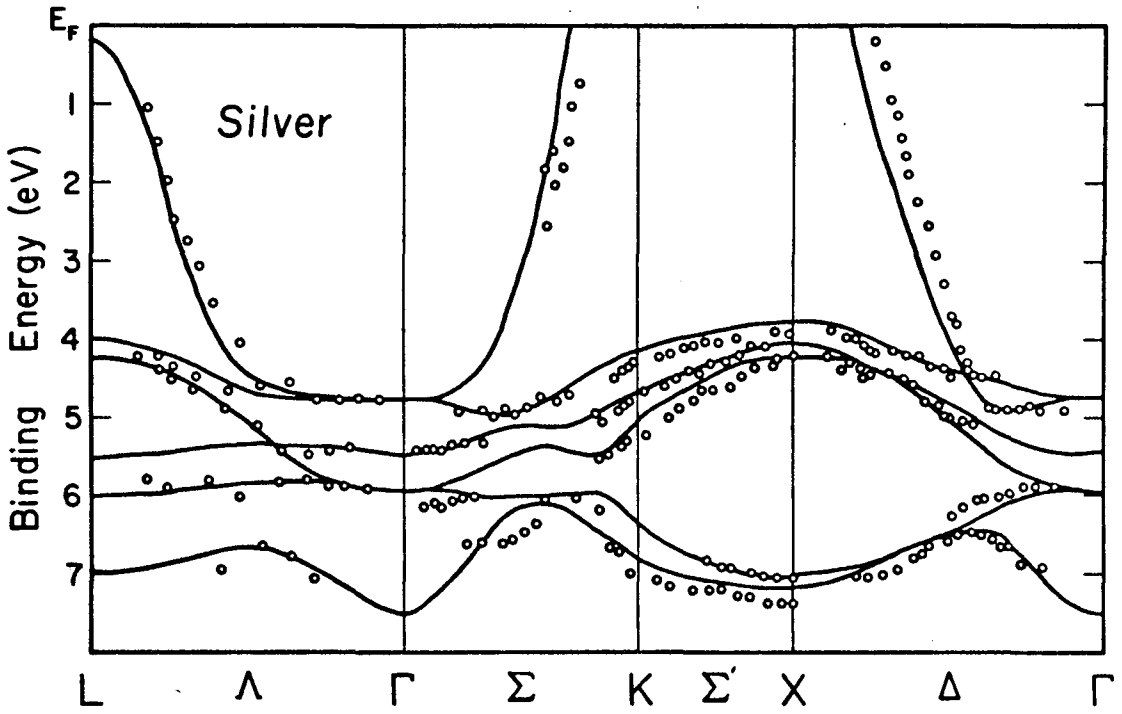

Figure 1. Experimentally derived band structure (circles) of silver. The RAPW bands (solid lines, Ref. 8) are shown for comparison. Data circles for the ΓΛL line are from Ref. 5.

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