

Response to "Comment on 'k-resolved inverse photoelectron spectroscopy and its application to Cu(001), Ni(001), and Ni(110)'"

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The main conclusions of our inverse photoemission work are unaffected by evidence of residual surface contamination because they are based on observations of energy dispersion and crude relative intensities of bulk-derived peaks. We suggest an alternative explanation of the new data of Dose, Glöbl, and Scheidt in terms of dipole selection rules and differences in experimental geometry.

The following two points need to be added to the Comment by Dose, Glöbl, and Scheidt.¹

(1) The new data of Ref. 1 do not alter the main findings and conclusions of our earlier papers.^{2,3} In those papers we reported the first experimental demonstrations of the use of *k*-resolved inverse photoemission to map $E(k)$ energy-dispersion relations for empty states in solids. The data analysis involved plotting *positions* of peaks associated with *bulk* direct transitions as a function of the parallel wave vector of the incident electrons. We also showed that the relative peak intensities as a function of both electron incidence angle and orbital character of the final state could be crudely understood in terms of theoretical momentum matrix elements which we calculated from the bulk band structure. Since our concern was with peak positions and crude relative intensities of bulk-derived features, our conclusions are not seriously affected by evidence of residual surface contamination.

(2) The demonstration in Ref. 1 that our Ni(001) surface was contaminated to the extent of 0.3 monolayer is not conclusive. Our apparatus did not have Auger monitoring capability, and so we cannot positively confirm or refute this assertion. We can, however, draw attention to the significantly different experimental geometries. In our normal incidence work we collected photons emitted within a finite solid angle centered about a nominal mean angle of photon emission $\bar{\theta}_p = 45^\circ$ with respect to the surface normal. The collection geometry in Ref. 1 is *azimuthally integrated*, and we estimate from their Fig. 1 that $\bar{\theta}_p = 50^\circ$. Appeal to the relevant dipole selection rules⁴ indicates that for higher values of θ_p we expect an enhancement of emission from transitions into the *s,p*-like states and a diminution of transitions into the *d*-like states. This would bring about a change of relative intensities in just the sense observed.

We can make a rough estimate of the effect by noting that the momentum matrix element vector for transitions into the *s,p* band is perpendicular to the surface, and should therefore couple into *p*-polarized photon emission with an intensity varying approximately as $\sin^2\theta_p$. Transitions into the *d* bands have transverse momentum matrix element vectors and can couple into both *s*-polarized emission (with no dependence on θ_p) and *p*-polarized emission (as $\cos^2\theta_p$). We can therefore expect the ratio of *s-p* intensity to *d* intensity to have an angular dependence resembling that of the function

$$R(\theta_p) = \sin^2\theta_p / (1 + \cos^2\theta_p) .$$

For the geometries specified above, we have $R(50^\circ)/R(45^\circ) = 1.25$. If we allow that $\bar{\theta}_p$ in our work was actually less than the nominal 45° , we have $R(50^\circ)/R(40^\circ) = 1.59$, $R(50^\circ)/R(35^\circ) = 2.11$, and so on. Deviations of this magnitude are quite within the bounds of possibility. Firstly, our detector subtends a large angle ($\sim 50^\circ$) at the sample and the response profile over its aperture is not known. Secondly, the source, sample, and detector are each mounted at relatively large distance from a separate flange, leading to the possibility of misalignments.

We cannot press this alternative interpretation much further at this stage since a proper comparison would require (a) knowledge of the response profile of our detector, and (b) inclusion of the reflecting properties of the collecting mirror in the instrument of Ref. 1, (c) a more quantitative estimate of the momentum matrix elements, and (d) a treatment of the way in which the electromagnetic fields (*s* and *p* components) change on crossing the sample surface. We can conclude however that polarization effects and differences in experimental geometry could account for a large part if not all of the differences reported in Ref. 1.

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¹V. Dose, M. Glöbl, and H. Scheidt, Phys. Rev. B **30**, 1045 (1984) (preceding paper).

²D. P. Woodruff, N. V. Smith, P. D. Johnson, and W. A. Royer, Phys. Rev. B **26**, 2943 (1982).

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⁴W. Eberhardt and F. J. Himpsel, Phys. Rev. B **21**, 5572 (1980).