Comments and Addenda

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Comment on the interpretation of the −3.3- and −2.8-eV features observed by Eberhardt and Plummer in Ni (001) photoemission

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We point out that Eberhardt and Plummer made a group-theoretical error in their interpretation of the feature they observed at −3.3 eV in their angle-resolved photoemission data from Ni (001). It cannot be due to a transition from an X_1 initial state into an X_5' final state as they have claimed. We also point out that the −2.8-eV feature they ascribe to an X_3 to X_5' transition can just as easily be interpreted to occur at W. These questions are important because of the controversy over the d-band width in nickel.

When the parameters of an angle-resolved photoemission experiment are such that $\vec{k}$ cannot be conserved (energy and $\bar{k}$, the transverse component of $\vec{k}$, are always conserved), the electronic transitions must occur in the surface region where $k_\perp$ is not a good quantum number. We[1] have recently shown that such was the case in the experiments of Lapeyre *et al.*[2,3] and that their data are in excellent agreement with the surface photoemission calculated from our[4] Ni (100) thin-film energy bands, which are based on the bulk Ni band calculation of Wang and Callaway[5] with a reduced-exchange splitting. Although the impressive bulk photoemission data of Eastman *et al.*[6,7] show a 30% reduction in the one-electron d-band width at the L point, the simplicity of interpretation of the surface photoemission data led us to favor the wider bands. This is an important controversy because of the large effort expanded[8-12] to show that the d-band narrowing of Ni is a many-body effect. Now Eberhardt and Plummer[13] (EP), also using bulk photoemission, have found results in general agreement with Eastman *et al.* although they differ in detail. (For example, at the bottom of the d bands, Eastman *et al.* find that $X_1 = -3.8$ eV, $L_1 = -3.4$ eV, whereas Eberhardt and Plummer find $X_1 = -3.3$ eV, $L_1 = -3.6$ eV.)

Although EP find nineteen occupied critical-point energies in the Ni bands, the only two for which they show their data and explain their interpretation are the X_1 and X_3 points at −3.3 eV and −2.8 eV. It is the purpose of this Comment to point out that the X_1 to X_5' transition that EP claim to see is strictly forbidden in the geometry they used. They had an (001) film with $\vec{k} = (2\pi/a)(1,0,0)$ and the vector potential $\vec{A}$ of the s-polarized incident uv radiation in the [100] direction. The only allowed transition from an X_1 initial state with this geometry is to an X_4' final state. With [010], radiation transitions to X_5' are allowed, but they are to the partner of the degenerate pair which is odd under reflection in the plane of emission and hence could not be detected.[14] Only with p-polarized [001] radiation could an X_1 to X_5' transition be observed. To obtain their X_3 peak, EP kept $\vec{A}$ fixed but rotated their detector by 90° so $\vec{k} = (2\pi/a)(0,1,0)$. This does give an allowed transition from X_3 to the even partner of X_5'; however, the transition could occur at any $\vec{k}$ vector of the form $(2\pi/a)(0,1,\alpha)$. In particular, a transition from W_3 to W_2' (which is even in the plane of emission) is allowed and would be in agreement with the one-electron energy bands.[5] Furthermore, if this were the X_3 level, a transition to the X_3' level at about[15] 42 eV should have been observed when they took $\vec{k} = (2\pi/a)(1,0,0)$. Thus we conclude that EP's interpretation of their −3.3-eV peak is incorrect and their interpretation of their −2.8-eV peak is open to question.

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