

Nahm *et al.* Reply: In the preceding Comment [1], Weightman *et al.* question the main conclusion of our Letter [2] that the discrepancy between photoemission spectra and theoretical density of states (DOS) of Cu₇₅Pd₂₅ is mostly caused by the matrix element effect rather than the lattice relaxation effect. They presented several arguments for this view, but as we will show below none of their arguments invalidates our conclusion.

(1) They argued that the inclusion of the matrix element effect alone cannot remove the discrepancy between experiment and theory for the x-ray photoelectron spectra of Pd [3], but that a complex self-energy broadening Σ alone can largely remove the discrepancy [4]. However, Fig. 7 of Ref. [4] clearly shows that there is still too much weight in the high binding energy region of the theoretical spectrum even after the self-energy broadening. This discrepancy can only be removed by the inclusion of *the matrix element effect as well as the lifetime broadening*, a procedure followed in our Letter [2] with the convincing result shown in its Fig. 2. This fact was pointed out even in Ref. [3], and the importance of the matrix element effect in Pd metal is unquestionable.

We agree that the transferability of Σ from pure metals to alloys is not guaranteed, but this is the best approximation we can make when there are no calculated results for Σ of Cu₇₅Pd₂₅. Weightman *et al.* worried about the possibility of the large $\text{Re}\Sigma$, but theoretically a large $\text{Im}\Sigma$ does not necessarily mean a large $\text{Re}\Sigma$. Furthermore, detailed studies on the electronic structure of Pd, Ir, and Pt revealed that even though $\text{Im}\Sigma$ is large, $\text{Re}\Sigma$ is negligible for the occupied states [5]. Weightman *et al.* also argued that the lifetime broadening for the alloy would be reduced due to the reduction of the Pd partial DOS (PDOS) at the Fermi energy. But the phase space for the decay of a *d* band hole is proportional to the total number of possible particle-hole excitations, and the PDOS at the Fermi energy has negligible influence on the lifetime of a hole with a large binding energy [6].

(2) They argued that the experimental photoionization cross section (σ) ratio of pure metals is not necessarily transferable to alloys, citing Ref. [7] which claimed to show that the photon energy dependence of $\sigma_{\text{Ag } 4d}$ changes appreciably from alloy to alloy. However, we have some reservations as to the validity of the analysis method employed in Ref. [7], since they normalized $\sigma_{\text{Ag } 4d}$ by the *atomic* cross section of Al *3p* and Cd *5s* states whose wave functions are expected to be influenced more by the solid state effect than for the Ag *4d* state. Even if we accept the conclusion of Ref. [7], it has little influence on our present analysis of Pd partial spectral weight (PSW) of Cu₇₅Pd₂₅ because of the negligible contribution of Pd states to the alloy photoemission spectra at the Pd Cooper minimum. We found that even if we increase $\sigma_{\text{Pd}}/\sigma_{\text{Cu}}$ at photon energy 130 eV from the original value of 0.03 to 0.15 (a 5 times increase), there is no appreciable change in the deduced Pd PSW.

(3) Lacking a theoretical calculation on the x-ray

emission spectra including self-energy corrections, this fact neither proves nor disproves our conclusion.

(4) The fact that the reduction of the theoretical Pd DOS at high binding energies by the lattice relaxation effect in Cu₇₅Pd₂₅ is not sufficient to bring agreement with experiment can be clearly seen in Fig. 3(b) of our Letter [2]. Even for the Pd impurity case, their claim that the local expansion can account for approximately half of the discrepancy is somewhat exaggerated since we believe the interatomic hopping matrix element of Ref. [8] is underestimated.

(5) The Auger spectra of Cu₇₅Pd₂₅ can only be fitted with the *empirical* Pd PSW with a reduced intensity at high binding energies. This suggests the importance of the matrix element effect in the Auger spectra as well, which generally reduces the contribution of high binding energy parts of *d* states to the Auger spectra as discussed in Ref. [2]. Also, the Pd Auger spectra of Mg-Pd, Al-Pd, and Ag-Pd alloys are inadequate examples for the present issue, since Pd PDOS in these alloys are quite narrow due to their split-band behavior and thus they are not strongly influenced by the change of the matrix element within the band unlike the Cu-Pd alloy case where the Pd PDOS is very broad.

In summary, we maintain that the discrepancy between experiments and theory on the Pd PDOS of Cu₇₅Pd₂₅ is essentially removed by the inclusion of the matrix element effect, and that our procedures are based on firm assumptions and do not leave any doubt for the dominating importance of the matrix element effect in this system.

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