Comment on "Experimental Evidence for One Highly Dispersive Dangling-Bond Band on Si(111)2 × 1"

Uhrberg *et al.*[1] conclude from their photoemission data that the dangling-bond surface states on Si(111) 2× 1 have to be interpreted as one band of states and not as two bands. We want to point out that the data in their paper are virtually identical to the data we have published previously[2] and cannot be used to distinguish between the two interpretations. For example, both data sets[1,2] show a dispersive upper state and a second lower state. Our conclusion is that the distinction between the two classes of current models for Si(111) 2× 1 (Ref. 3 and Refs. 4–6, respectively) will require different types of experiments or different photoemission data.

In the band dispersion in Ref. 2, the two surface features are separated the farthest at the $\bar{J}$ point where one state is seen as a peak at E_v − 0.15 eV and the second state as shoulder around E_v − 0.7 eV. In agreement, the data of Ref. 1 show these same features, i.e., a strong peak at E_v − 0.10 eV and a weak peak at E_v − 0.75 eV. The intensity (i.e., the area) of the weaker peak in Ref. 2 is very similar to the intensity of the shoulder seen in Ref. 1 whether normalized to the bulk, to the lower state at $\bar{\Gamma}$, or to the upper state at $\bar{J}$. Uhrberg *et al.*[1] dismissed this structure by comparing with multidomain cleaves which can cause its intensity to become increased. Previously, we found that such multidomain cleaves resulted in irreproducible intensities for the two peaks in question. Rather than relying on multidomain-cleave data, as done in Ref. 1, one can use the best single-domain–cleave data and come to the opposite conclusion; i.e., the extra lower peak (reproduced in Ref. 1) is an intrinsic feature of the Si(111) 2× 1 cleavage surface.

Concerning $E(\vec{k})$ band dispersions, our original data set (see Fig. 3 in Ref. 2) and the data set of Uhrberg *et al.* yield $E(\vec{k})$ dispersions which agree to within 0.07 eV for all $\vec{k}$ points if *peak* positions[1] are used to derive $E(\vec{k})$. We resolved our spectra into two peaks, giving a slightly smaller but perceptible dispersion with the largest $E(\vec{k})$ discrepancy occurring at $0.75(\bar{\Gamma}\text{-}\bar{J})$, where both data sets show the *same* (within 30 meV) peak position.

We conclude that the available photoemission data cannot support or eliminate either of the two types of current models for Si(111) 2× 1. Both possibilities were used for the discussion in our previous paper.[2] For example, if the one-band interpretation[3] is correct, then the lower peak[1,2] indicates that the number of defects on the Si(111) 2× 1 cleavage plane cannot be reduced below a certain limit, at least in all photoemission experiments to date. This could be an intrinsic property of this metastable surface, e.g., a stabilization by steps.[5] Alternatively, it is quite possible that there are two excited surface-state levels, as we have previously discussed, based on extensive two-dimensional angular-emission data.[2,6] Correlated antiferromagnetic band calculations[4,5] give nearly flat bands, while a fully correlated cluster calculation by Redondo *et al.*[6] gives two bands, with a strong dispersion of the upper state that is similar to the experimental data in Refs. 1 and 2.

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[1]R. I. G. Uhrberg, G. V. Hansson, J. M. Nicholls, and S. A. Flodström, Phys. Rev. Lett. 48, 1032 (1982).
[2]F. J. Himpsel, P. Heimann, and D. E. Eastman, Phys. Rev. B 24, 2003 (1981).
[3]K. C. Pandey, Phys. Rev. Lett. 47, 1913 (1981).
[4]R. Del Sole and D. J. Chadi, Phys. Rev. B 24, 7431 (1981).
[5]J. E. Northrup, J. Ihm, and M. L. Cohen, Phys. Rev. Lett. 47, 1910 (1981).
[6]A. Redondo, W. A. Goddard, III, T. C. McGill, F. J. Himpsel, and D. E. Eastman, to be published.