Comparison between some recent W(001) surface-state resonance studies above the vacuum level

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Comparison is done between a recent high-resolution study of low-energy-electron diffraction threshold effects and a recent theoretical calculation on the same phenomena. Some comments related to other recently published works are proposed.

We have recently published an experimental high-resolution study of low-energy-electron diffraction (LEED) threshold effects on the W(001) surface.[1] New sharp features have been detected in the I-V curves and correlated with the emergence condition of the first nonspecular diffracted $(\bar{1}0)$ beam. Two possible interpretations were proposed: the two narrow dips B and C are the $n=2$ and $n=3$ members of a surface-state resonances series, the $n=1$ member being the feature seen in previous measurements,[2] or their origin may be explained by a true threshold effect. In conclusion we outlined the need for other studies and specially for high-resolution calculations on surface resonances or threshold effects. During the time our article was in press, such a new high-resolution calculation was reported.[3] It is the purpose of this short comment to compare these very recent theoretical results with some points of our experimental study. The theory predicts a Rydberg-like spectrum of surface resonances just below the emergence of each new nonspecular beam diffracted from a metal surface. The levels are given by

$$E_n = -\tfrac{1}{16}\,[1/(a+n)^2]\ \mathrm{Ry}\,, \qquad (1)$$

where $\frac{1}{16}$ is a constant theoretically determined and a should lie between 0 and 1. We have tried to fit the position of the minima A, B, and C (Fig. 1 of Ref. 1) with this equation, for five incident angles corresponding to threshold energies between 4.7 and 5.05 eV (Fig. 3 of Ref. 1). n values 1, 2, and 3 are assigned to features A, B, and C, respectively. From the experimental $\Delta_{21}=E_2-E_1$ values and from Eq. (1), a is calculated taking into account the uncertainty in the position of the A and B minima; the expected spacing $\Delta_{32}=E_3-E_2$ is then calculated. The results are summarized in Table I.

It can be seen that the agreement between the predicted and the observed series is satisfactory and the parameter a lies effectively in the expected range $0<a<1$ (another real negative root is obtained from Δ_{21} but gives Δ_{32} values very far from the experimental ones).

The five sets of experimental points seem thus to support quite strongly the theoretical predictions about a Rydberg-like series of surface resonances near the nonspecular beam threshold energy. In the case of the two other incident angles for which we have detected three dips, the positions of these dips do not obey the same equation. This is perhaps related with the observed vanish-

TABLE I. For five incident angles, range of values for the constant a, the calculated and the observed Δ_{32}.

Values of a from $\Delta_{21}=E_2-E_1$	$0.073<a<0.121$
Calculated values of $\Delta_{32}=E_3-E_2$	$0.102<\Delta_{32}<0.108$ (eV)
Observed values of $\Delta_{32}=E_3-E_2$	$0.095\pm0.006<\Delta_{32}<0.101\pm0.006$ (eV)

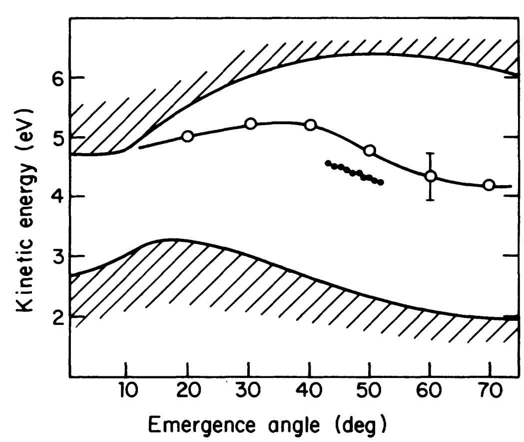

FIG. 1. Angular behavior of the surface resonance; circles and line: experimental SEE peak, and shaded regions: bulk bands, both results taken from Fig. 2 of Ref. 4; dots: our experimental (LEED) results obtained from the data on Fig. 3 of Ref. 1: the dots reported here are the minima of the first resonance profile (feature A of Ref. 1).

ing of dip C for $\theta_i < 45°$. The observed disappearance of the well-defined dips B and C for $\theta_i < 45°$ and $\theta_i > 51°$ does not seem to emerge naturally from the proposed theory.[3]

We want to add a few other comments on the comparison of our results with another very recent study by secondary electron emission[4] (SEE). In this work, strong emission from a state lying in the bulk band gap was observed; the dispersion $E(\theta)$ of this state is in agreement with the dispersion $E(\theta)$ of our feature A in the region near 45°. Comparison between our results and the results of of SEE[4] is displayed in Fig. 1 (the SEE results were compared[4] with a calculation by Smith and Mattheiss[5]). In view of the agreement shown in Fig. 1, it is tempting to identify both experimental features. This fact is important since it is a reconciliation of the LEED and of the band structure approaches of the surface resonance effect: the surface resonance (or surface state resonance, or unbound state or quasistationary state) is effectively seen not only in the elastic (LEED) channel but also in a channel more sensitive to electronic structure (SEE); the fact it should be so was outlined by Hoffstein.[6]

Finally we feel that, in view of this relation it would be very interesting to look for fine structure near the emission peak seen in SEE[4] with a total resolution equal to (or better than) 15 meV; this resolution was found necessary[1] to resolve the tentatively assigned $n = 2$ and 3 members of the Rydberg-like resonances series.[3]

[1]A. Adnot and J. D. Carette, Phys. Rev. Lett. 38, 1084 (1977).
[2]E. G. McRae and G. H. Wheatley, Surf. Sci. 29, 342 (1972).
[3]J. Rundgren and G. Malmström, Phys. Rev. Lett. 38, 836 (1977).
[4]R. F. Willis, B. Feuerbacher, and N. E. Christensen, Phys. Rev. Lett. 38, 1087 (1977).
[5]N. V. Smith and L. F. Mattheiss, Phys. Rev. Lett. 37, 1094 (1976).
[6]V. Hoffstein, Surf. Sci. 33, 345 (1972).