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High-Resolution Study of Low-Energy-Electron-Diffraction Threshold Effects on W(001) Surface

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The simultaneous high-energy-resolution and high-angular-resolution (15 meV, 0.8°) measurements of the (00) beam diffracted from W(001) near 45° incident angles are reported. Apart from the well-known surface-state resonance previously identified, new features located in the close vicinity of the $(\bar{1}0)$ emergence energy are detected. They may remain undetected if one of the two high-resolution requirements is not fulfilled. The threshold effects are correlated with the $(\bar{1}0)$ beam emergence by angular distribution and I-V measurements, and possible interpretations are discussed.

The needs for high-resolution low-energy-electron-diffraction (LEED) experiments have been stressed by numerous authors: The knowledge of the exact position and shape of the surface-state resonances is of primary importance for the determination of the surface-potential-barrier parameters[1-5]; high-resolution measurements can help to make the distinction between surface-state resonances and beam threshold effects[6] and to clarify the origin of some singularities[7,8] in I-V curves; the limited resolution of conventional LEED equipment may blur[5] fine details of I-V curves; indeed, a sharp and highly localized effect just at the detection limit imposed by a 0.4-eV resolution has been recently reported.[7]

Working at very low energy presents the advantage that the dynamical effects for the first non-specular diffracted beams are located below the strong inelastic surface and volume-plasmon thresholds. This inelastic scattering attenuates, broadens, and displaces the features.[9] Thus it becomes more difficult to determine true shape and position of the details, in the absence of a quantitative theoretical treatment of the adsorptive part of the potential. To our knowledge only one experiment[10] has so far been reported in the low-energy range with a 70-meV resolution at 53° incidence angle. The angular resolution was not given. It has been analyzed by many other autors.[5,9,11-13]

We report in this Letter the study of the (00) beam diffracted from W(100) for incidence angles near 45°, a 15-meV energy resolution, and an angular detector resolution better than 0.8°. This performance has permitted the detection and identification of new features whose widths are more than one order of magnitude smaller than any of the singularities reported thus far in LEED I-V curves. The apparatus used is a tandem of 127° electrostatic electron spectrometers. The general arrangement is the same as that used in former experiments,[14] except that a new monochromator and lenses have been mounted. Design details of these electrostatic spectrometers have been fully described elsewhere.[15] The analyzer may be roted in the incidence plane so that angular measurements are possible. The stated 15-meV resolution is the masured full width at half-maximum (FWHM) of the reflected (00) beam and 0.8° is the measured angular FWHM using a 30-eV well-focused beam. Orientation of the (001) face is good within $\frac{1}{2}$° as checked by x-ray diffraction; the crystal is oriented so that the incidence plane contains the [10] direction (azimuthal angle $\varphi = 0$) within $\pm\frac{1}{4}$°. The crystal has been submitted to standard oxygen treatment, and a stable, clean, and reproducible surface is obtained by flashing at 2400°K in the UHV system with a base pressure of 2×10^{-11} Torr. Auger analysis of the residual surface impurities is not possible, but surface quality was checked in a separate experiment with the same apparatus by observing the high-contrast (10) beam and the 4×1 pattern associated with low-coverage oxygen adsorption.[16] Severe experimental precautions are taken to insure that the results are free from contamination and temperature effects.

The study of correlation between observed features in the I-V curves and beam-emergence conditions requires the variation of at least one of the two impact angles. As in our apparatus neither the incidence nor the azimuthal angle can be changed from outside the vacuum system, we worked with a defocused primary beam, so that a large distribution of incident angles is available. Moving the analyzer permits choice of an effective incident angular slice whose width is evidently equal to the analyzer angular resolution. An incident defocused beam of $\simeq 8°$ total angular width was used in the 3–7-eV energy range.

Figure 1 shows the (00) I-V curve for an analyzer position of 48° with respect to the surface normal. Three dips labeled A, B, C, and a sharp slope discontinuity D are clearly visible. The dip widths Γ measured between the bottom of the dip and the nearest maximum on the high-energy side are $\Gamma(A) = 365$ meV, $\Gamma(B) = 63$ meV, $\Gamma(C) = 19$ meV. If these features are correlated with the $(\bar{1}0)$ beam grazing emergence condition, they should be observed in angular distribution

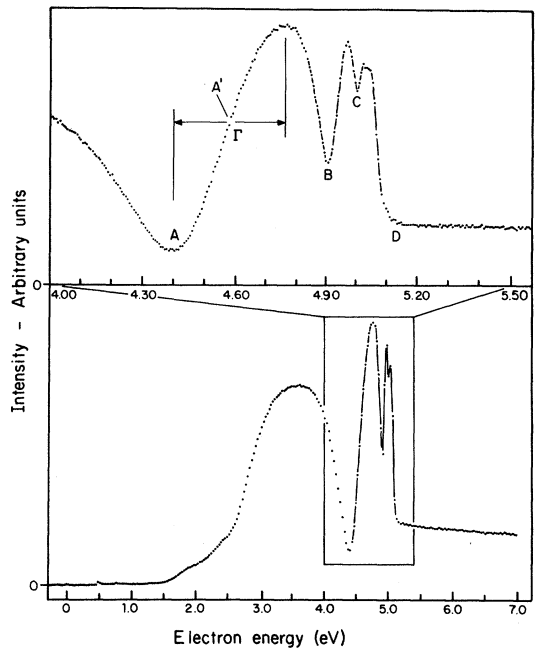

FIG. 1. I-V curve of the (00) beam for two energy scales. Incidence angle (or analyzer position) is 48°. Γ and A' are width and center of feature A according to the definitions of Ref. 13.

measurements, their angular position should change with incident energy, and their angular widths should be roughly proportional to their energy widths. This behavior is shown in Fig. 2 for the features B and C. Angular study of feature A has been done too, but is not shown here (it corresponds to the dark-band observation of Ref. 13). Figures 1 and 2 clearly show that if either energy or angular resolution is not sufficient, features B and C escape detection in the two measurements simultaneously.

A systematic study of the features position E_0 as a function of incidence angle θ_i (or analyzer position) has been performed with a series of I-V curves; the results are displayed on Fig. 3, where E_0 is plotted in terms of $E_T - E_0 = f(E_T)$, where E_T is the calculated $(\bar{1}0)$ emergence energy. Position and behavior of feature A are in good agreement with previously published results[13]; this confirms that our estimation of the uncertainty on the incident energy (50 meV) is good. Its identification with the surface-state resonance is unambiguous and will not be discussed further here. We only point out that its width is lower than the reported values of 1 eV (Ref. 13) and 0.6 eV (estimated from Propst and Edwards curve given in Ref. 13). By comparison, the new features B and C exhibit a very different

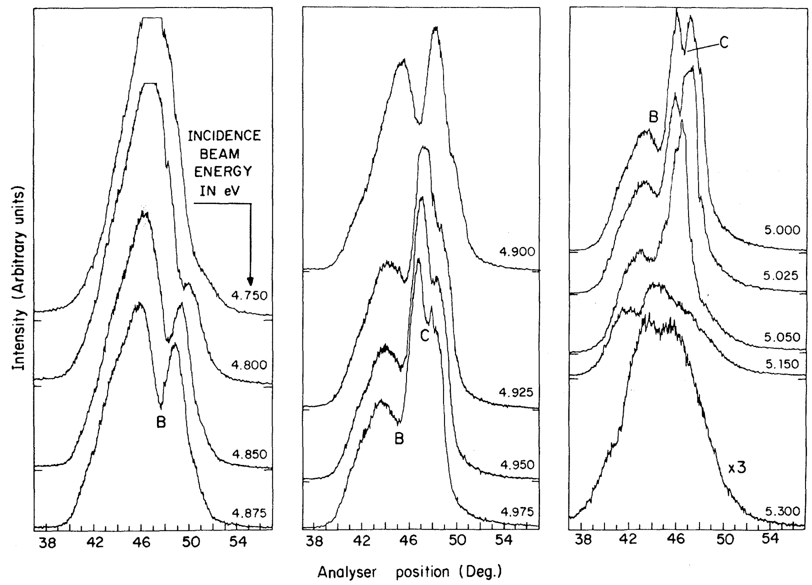

FIG. 2. Angular distribution of the (00) beam for various incidence energies. The noise is the sum of statistical noise and microphonic noise induced by analyzer rotation.

behavior. They are located in the band $E_T - E_0 \simeq 0 \pm 0.125$ eV. For $\theta_i < 45°$, arrow b in Fig. 3, only dip B is present but its intensity is much lower than for $\theta_i > 45°$. For $\theta_i > 52°$, arrow a in Fig. 3, B and C disappear. So it seems that B and C are localized near $\theta_i = 45°$. It has recently been proposed[17] that a serires of surface-state resonances converging to the emergence energy

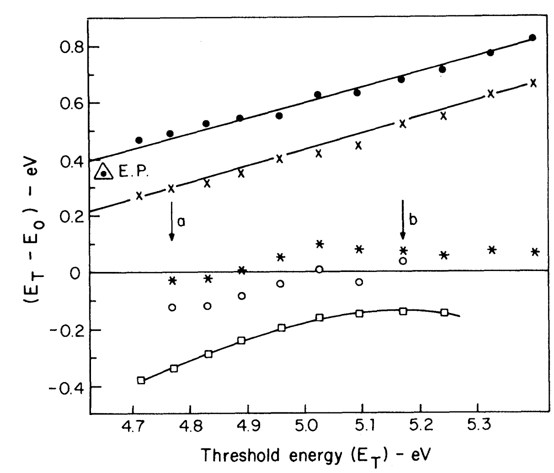

FIG. 3. Correlation of feature position E_0 with calculated $(\bar{1}0)$ threshold energy (E_T) expressed in terms of $(E_T - E_0) = f(E_T)$. ×: point A' (see Fig. 1); •: dip minimum A; ∗: dip minimum B; ○: dip minimum C; □: slope discontinuity D. Point △ refers to the position of point A' in the curve of Edwards and Propst given in Ref. 13. At left from arrow a, the dips B and C disappear, at righ from arrow b, only B is detected (see text).

of the diffracted beam might be present. The features A, B, and C may be the first three members ($n = 1, 2, 3$) of such a series, and the decreasing of the width as n increases is observed, as expected.[17] It is, however, not clear why the $n = 2$ and 3 members are detected only near 45°, while the $n = 1$ resonance extends over a large angular range, from $\theta_i = 16°$ to at least $\theta_i = 53°$.[13] An alternative interpretation is that feature B and C are the manifestation of a true threshold effect just at the vacuum emergence of the $(\bar{1}0)$ beam. Such a condition should lead to fluctuation in the (00) beam because the electrons which are now outside the crystal can no longer contribute to the (00) intensity and the width of the associated fluctuation can be much less than the surface resonance width.[7] Single dips located at the emergence energy of nonspecular beams have been observed in a number of cases,[8] however, without systematic study of their position with varying θ_i. A more interesting case has been recently reported on Al(100)[7] where a relatively sharp and highly localized effect has been detected; it seems to occur at the grazing emergence energy of the four (11) beams; its strong dependence on orientation is not expected on the basis of superposition of beam threshold effects, but is expected if one assumes that the threshold effect itself is localized in a narrow region about a preferred direction, namely the normal to the surface in this case. Thus on the basis of this result, the interpretation of features B and C as being the manifestation of a threshold effect localized near $\theta_i = 45°$ is not unlikely. It has been suggested[9] that singularities at threshold energies (vacuum branch points) should be detected as slope discontinuities in the I-V curves. Feature D (Fig. 3) shows a less definite correlation with the threshold condition $E_T - E_0 = 0$ than B and C. The interpretation in terms of a true threshold effect, however, does not explain why two dips are observed. The physical nature of our observations remains somewhat unclear but those new results demonstrate the usefulness of high-resolution electrons spectrometry applied to diffraction experiments; it is hoped that they will stimulate other high-precision experimental studies and theoretical calculations about surface resonances and threshold effects.

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Surface Resonance Bands on (001)W: Experimental Dispersion Relations

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A band of unbound surface states (resonances), located in an energy region above the vacuum threshold corresponding to an energy band gap in the electron states of the bulk crystal, has been observed by angle-resolved secondary-electron-emission spectroscopy. The experimental dispersion behavior is in agreement with the two-dimensional band structure of a clean (001)W surface recently proposed by Smith and Mattheiss.

The two-dimensional band structure for the prominent surface states/resonances associated with the clean (001)W surface, and that for a saturation coverage of chemisorbed H atoms, have recently been determined by a parametrized linear-combination-of-atomic-orbitals (LCAO) slab-model calculation.[1] The calculated energy versus parallel wave-vector (E vs $\vec{k}_{\parallel}$) relations permit an identification of spectral features observed in angle-resolved photoemission measurements.[2,3] In particular, the LCAO calculation predicts a band of unbound states located a few eV above the vacuum threshold, E_{vac}, which gives rise to structure appearing in the inelastic or secondary-electron part of the photoemission spectrum,[3] the latter reflecting the electronic energy band struc-