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Energy- and angular-dependent secondary-electron emission from a silicon (111) 7×7 surface. II. Emission from surface-state resonances

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Secondary emission spectra from surface-state resonances in the $[2\bar{1}\bar{1}]$ and $[11\bar{2}]$ azimuths of the silicon (111) 7×7 surface are discussed. The spectra extend to 6 eV above the vacuum level, with resonances with $k_{\parallel}=0$ occurring at energies of 0.87 ± 0.01 eV, 1.15 ± 0.02 eV, and 3.5 ± 0.1 eV above the vacuum level.

I. INTRODUCTION

When a low-energy (< 300 eV) beam of electrons strikes a silicon (111) 7×7 surface the resulting secondary-electron emission can be categorized in one of two types: emission of electrons which initially had been excited into bulk-conduction states, or emission of electrons which initially had been excited into surface-state resonances. It is possible to find incident-beam conditions which enhance the intensity of one type of emission relative to the other, allowing each of the two types of emission to be studied separately, more or less. In part I of this series the energy and angular dependence of secondary-electron emission (EADSEE) from bulk states was reported and discussed.[1] This paper deals with EADSEE from surface-state resonances.

EADSEE for electrons emerging from surface-state resonances in the $[2\bar{1}\bar{1}]$ azimuth of this surface were reported earlier.[2] Peaks in the spectra observed at angles of emergence of from 60° to 90° with respect to the surface normal were interpreted by a two-step analogy of the normal three-step model used to describe secondary emission from bulk states: electrons are excited from occupied states into surface-state resonances, from which they emerge into the vacuum. These data yield information about the final states. There is no "memory" of the initial occupied state, and here the excitation process itself is only probed to the extent that incident beam conditions which enhance the emission from surface-state resonances are reported.

For electrons coherently crossing an ordered two-dimensional surface energy is conserved, and

$$k_{\parallel\,\mathrm{out}}=k_{\parallel\,\mathrm{in}}+b_{\parallel}\,,$$

where $k_{\parallel}$ is the component of the wave vector parallel to the surface, and $b_{\parallel}$ is one of the set of surface reciprocal-lattice vectors.[3] A peak at kinetic energy E in the emission spectrum at emergence angle θ was taken to imply the existence of a surface state resonance at energy E, and a $k_{\parallel}$ given by

$$k_{\parallel}=\sqrt{2E}\sin\theta+b_{\parallel}\,, \tag{1}$$

where E is in atomic Hartree units ($\hbar=m=e=1$), referred to the vacuum level as origin. The dispersion curves of the surface-state resonances were thus deduced from the data, and compared with those calculated on the two-dimensional ($2D$) free-electron model described by McRae[4]:

$$E(k_{\parallel})=K_v^2+(M_1a_1+M_2a_2+k_{\parallel})^2\,, \tag{2}$$

where K_v is a constant, M_1 and M_2 are integers, and a_1 and a_2 are basic surface reciprocal-lattice vectors. The details of that comparison are described here, as they were not included in the earlier work. Also in the present paper the EADSEE spectra recorded in the $[11\bar{2}]$ azimuth of a silicon (111) 7×7 surface are presented and discussed, and a brief comparison made between EADSEE from reconstructed and unreconstructed surfaces, respectively.

II. RESULTS AND DISCUSSION

First, the discussion of the results for the $(2\bar{1}\bar{1})$ surface, presented previously,[2] will be completed. Dispersion curves of E vs $k_{\parallel}$ as deduced previously are shown as dots in Fig. 1, where the 2D free-electron surface bands [Eq. (2)] are shown by solid lines.

The points from A to B to D in Fig. 1 appear to belong to a free-electron band structure. On this basis a fit between free-electron dispersion curves and the experimentally derived points was attempted. The only adjustable parameter was the energy at which experimental point B should be matched to the free-electron curve. It was noted that theory shows that real dispersion curves repel each other,[4] so in this fitting the degree of separation

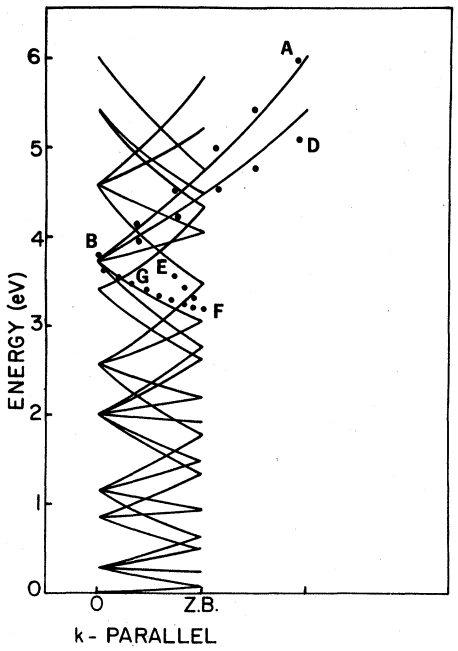

FIG. 1. Dispersion curves for resonances observed by secondary electron emission in the [2$\bar{1}$1] azimuth of the silicon (111) 7×7 surface. The points are from the experimental measurements (Ref. 2), while the solid curve is the 2D free-electron dispersion curve for surface-state resonances, calculated as described by McRae (Ref. 4). The zero of energy in this figure is deduced to be 2.5 ± 0.1 eV below the vacuum level.

between the experimental branches *AB* and *BD*, respectively, should be greater than that between the corresponding free-electron curves. Fitting *B* at the branch point at 4.6 eV actually gave better agreement between theory and experiment than for the match shown in Fig. 1. That fit was rejected, however, because the 2*D* free-electron curves diverged slightly more rapidly than did the lines *BA*, *BD*, respectively. At higher and lower energies a much worse fit was obtained.

Knowing the energy of point *B* above the vacuum level from the measurements, and the ionization potential of this surface from photoemission data,[5] it was possible to deduce that the bottom of this free-electron band of surface states was 2.5 eV above the top of the valence band. This assignment has received support from other studies. Measurements of the angular dependence of inelastic electron scattering indicated that the bottom of the surface conduction band is 2.3 ± 0.2 eV above the top of the valence band,[6] and, in a related calculation, of the surface band structure of silicon (111) 1×1 surface, Schlüter and Cohen deduced that the bottom of the surface band is at 2.8 eV above the top of the valance band.[7,8]

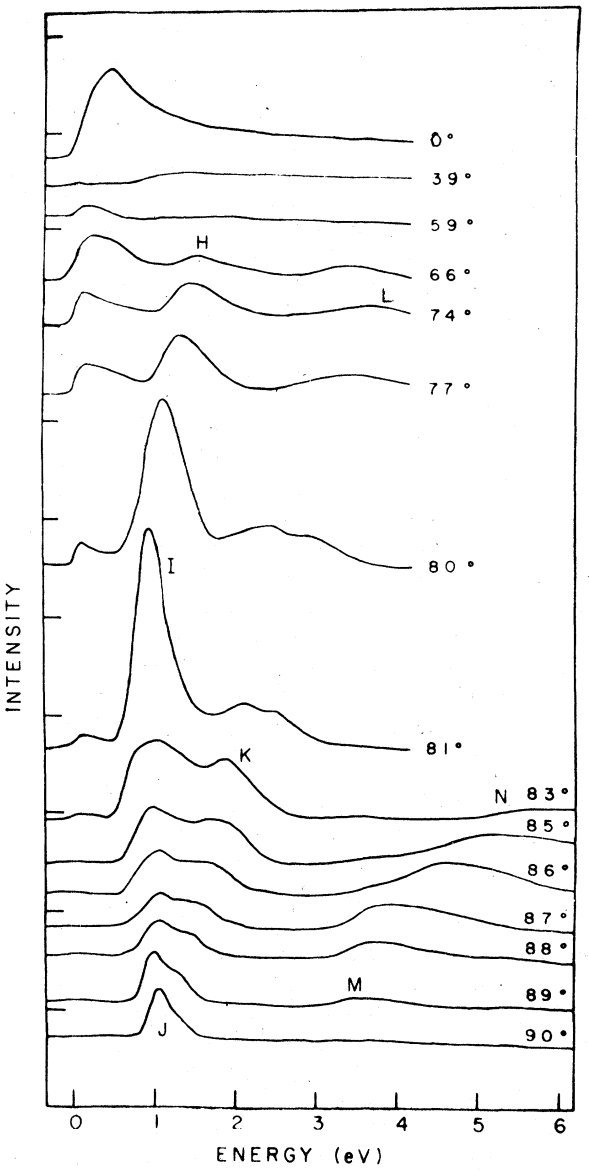

FIG. 2. Secondary-emission spectra measured in the [11$\bar{2}$] azimuth of silicon (111) 7×7. Energy is measured relative to the vacuum level, taken from the inflection point of the initial rise of the 0° spectrum, angles being measured from the surface normal. The intensity of the spectra at 0°, 39°, and 59° have been reduced by a factor of 10 relative to the other spectra.

The new EADSEE results reported here are for the [11$\bar{2}$] azimuth of the silicon (111) 7×7 surface prepared as described previously.[2] For constant input beam conditions, an energy of 50 eV at a polar angle of about 20° in the [$\bar{1}$1$\bar{2}$] azimuth, the energy spectrum was recorded at each angle of emergence at 1° intervals. A selection from a typical series of spectra is shown in Fig. 2. The

series of peaks extending from that labeled H, through I, J, and K to L, and between M and N, respectively, are the ones believed to be associated with emission from surface-state resonances. While the peaks from H to I are single valued, from K to L some double-peaked structures are observed. The low-energy peak in the spectra from 0° to 81° from the surface normal is believed due to emission from bulk states, as described previously.[1]

Points on the surface-state-resonance dispersion curves deduced from the positions of the observed peaks by Eq. (1) are shown as dots in Fig. 3,

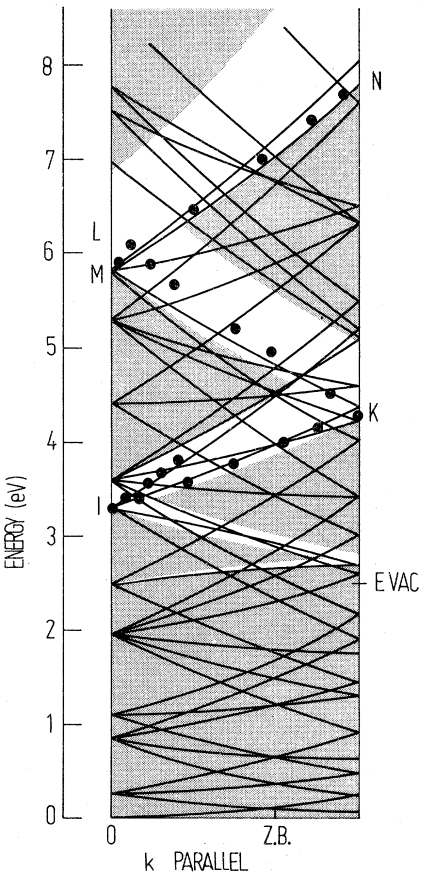

FIG. 3. Dispersion curves for resonances observed by secondary electron emission in the [11$\bar{2}$] azimuth of the silicon (111) 7×7 surface. The points are deduced from the data of Fig. 2, as described in the text; the solid lines are the 2D free-electron dispersion curves for surface-state resonances (Ref. 4). Resonances in the unshaded areas are the only ones which can emerge into the vacuum at angles between 60° and 90° from the surface normal. Secondary emission features corresponding to surface-state resonances have only been observed at angles greater than 60° for spectra from this reconstructed silicon surface.

where the 2D free-electron bands, calculated as described by McRae[4] [Eq. (2)], are shown by the solid lines. For the [11$\bar{2}$] azimuth there is no parameter to adjust in the comparison between experiment and theory (Fig. 3). There is good agreement between experiment and simple theory.

When compared with the 2D free-electron calculations, and with each other, there are two types of apparent inconsistencies in the data from the two azimuths. The first is that many free-electron states are predicted where no resonances are observed. This is not particularly troublesome, as there are not sufficient calculations of bulk band structure available to determine which of the calculated states may occur as resonances.[4]

The other problem is that resonances close to the center of the zone are observed at 0.95 ± 0.1 eV for the [11$\bar{2}$] azimuth, and 1.1 ± 0.1 eV for the [2$\bar{1}\bar{1}$]. From energy considerations alone it could be claimed that these are one and the same resonance. We will discuss why it is probable that two different resonances are being observed, and why only one of them is observed in each azimuth.

In the deduced value of $k_{\parallel}$ for a peak there is considerable error, most of it coming from uncertainty in the determination of the kinetic energy [Eq. (1)]. We suggest a way around this problem, based on the observation that in a series of peaks in secondary spectra, such as those from H to J in Fig. 2, the peak of noticeable maximum height has a deduced $k_{\parallel}$ value which is very close to the center of the reduced zone. The intensity of members of this series, relative to one another, is independent of the incident-beam conditions, even though the overall visibility of the series depends on those conditions.

If the incident beam causes the resonances to be occupied according to their local density, as is the case for bulk states,[9] then the largest peak of a series will be associated with resonances at critical points in the zone, such as at the center or at boundaries. We then assume that the largest peak (e.g., I of Fig. 2), corresponds to resonances with $k_{\parallel} = 0$ in the reduced-zone scheme, similarly for the peak corresponding to point B in Fig. 1. In further support of this assignment it is observed that the peak of greatest intensity has the lowest energy of a series: such turning points commonly occur at critical points in the zone. While we previously used observed values of E and θ to calculate $k_{\parallel}$ from Eq. (1), now we use the observed value of θ for a resonance at a known value of $k_{\parallel}$ ($k_{\parallel} = 0$, identified as described above) to calculate the corresponding value of E, also by Eq. (1). The accuracy of the measured energy of a peak is sufficient to unambiguously determine $b_{\parallel}$ in Eq. (1). The accurate angular information (±2°) can then

be used to calculate the kinetic energies of the electrons emerging from resonances having $k_{\parallel} = 0$; $E = 1.15 \pm 0.02$ eV for the peak observed in the data from the $[2\bar{1}\bar{1}]$ azimuth, and $E = 0.87 \pm 0.01$ eV for that in the $[11\bar{2}]$ azimuth: There are apparently two distinct resonances. Because the emergence can be accompanied by diffraction, electrons of energy 1.15 eV could emerge at angles of 0°, 30°, and 79° in the $[2\bar{1}\bar{1}]$ azimuth, and at 0° and 58° in the $[11\bar{2}]$; the 0.87-eV electrons could emerge at 0° and 34° in the $[2\bar{1}\bar{1}]$ azimuth, 0° and 81° for the $[11\bar{2}]$. Peaks are not observed at all of these angles (see Fig. 2 for the $[11\bar{2}]$ azimuth).

The relative probability for electrons to emerge at angles allowed by the conservation laws is determined by wave-matching conditions across the interface.[10] The overall visibility of a peak in the secondary spectra will depend on the occupancy of the associated resonance, and the emergence probability, as well as the background due to secondaries emerging from bulk states. In the secondary spectra observed from reconstructed surfaces so far no peaks associated with surface resonances have been observed at angles of emergence of less than about 55°, suggesting that a combination of the above-mentioned factors precludes such observation. It is probably for reasons like this that evidence for only one $k_{\parallel} = 0$ resonance, in the energy region of 1 eV, is observed in the spectra from each azimuth, when at least two exist.

We can use the conservation laws to relate the values of E and $k_{\parallel}$ for electrons emerging into the vacuum for angles between 60° and 90°. The corresponding resonances lie in the unshaded region of Fig. 3, and are the only ones observed.

Secondary emission from resonances in unreconstructed tungsten surfaces have been reported and discussed in detail by Willis *et al.*[11] In those cases there was little incoherent scattering as electrons from bulk states emerged into the vacuum, and the effects of band gaps in the bulk electronic distribution were reflected in the emission spectra as pronounced dips in the secondary current.[12] Emission from surface-state resonances appeared as peaks in that dip, corresponding to the presence of the resonances within the band gaps.[11] Those spectra are quite distinct from the ones reported for the reconstructed surface. Considerable scattering of electrons, as they emerge from bulk to vacuum states, for the most part obscures the effects of bulk band structure on the emission spectra.[1] Emission from surface-state resonances is observed only for large angles from the surface normal, under incident-beam conditions for which emission from bulk states is a minimum.

An extensive study of secondary spectra from the vacuum level up to 20 eV was made in both the $[2\bar{1}\bar{1}]$ and $[11\bar{2}]$ azimuths of this silicon surface. No features, other than the ones identified here, could be associated with surface-state resonances.

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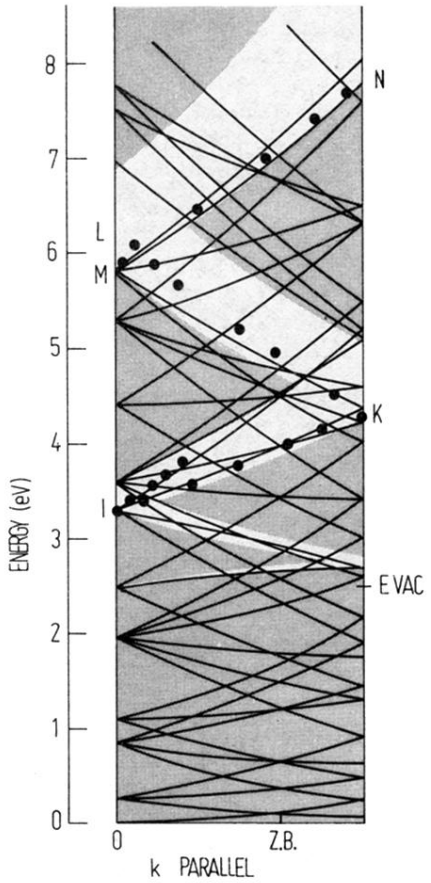

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