

clusion from an analysis of photoemission data.

⁷The SEE spectra were insensitive to variations in polar angle θ , or azimuthal angle φ , up to 5° off normal direction at the crystal face. The spectra were, however, found to be extremely sensitive to strong electrostatic patch-field effects in the vacuum chamber, particularly those features appearing at $E_k \lesssim 10$ eV. These effects could be balanced by the careful adjustment of a small negative potential, $V_s \simeq -0.75$ V, on the target crystal.

⁸N. E. Christensen and B. Feuerbacher, Phys. Rev. B **10**, 2349 (1974); N. E. Christensen, unpublished.

⁹Evidence to support a correlation between maxima in SEE spectra and density-of-final-states fine structure for energies $E_k \gtrsim 10$ eV has been published [see Refs. 2 and 3].

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¹⁶Preliminary results on the variation of secondary-electron spectra with polar angle $0 < \theta < 70^\circ$ have been presented; R. F. Willis, in Proceedings of the Fourth International Conference on Vacuum Ultraviolet Radiation Physics, Hamburg, Germany, July 22–26 1974 (to be published).

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Angle-Resolved Secondary-Electron-Emission Spectra from Si(111)7 × 7 Surface States*

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In angle-resolved secondary-electron-emission spectra from a silicon (111)7 × 7 surface there are two series of peaks which are not in the spectra of the unreconstructed (111)1 × 1 surface. These peaks are interpreted by a two-step model; electrons are excited into surface-state resonances lying above the vacuum level, from which states they emerge into the vacuum. The dispersion curves of these states are presented and discussed.

Measurements of the energy and angular dependence of secondary-electron emission (EADSEE) are made to gain a more detailed understanding of all the processes involved in the emission. Previous measurements have yielded data that fall into two classes: structureless spectra whose intensity at any one energy varies as the cosine of the angle between the direction of emergence and the surface normal¹; or structure other than this, which has been related to features in the density of bulk electronic states.² Here I report a high-resolution study of EADSEE from a single-crystal Si(111)7 × 7 surface.

The apparatus consists of an electron monochromator source, fixed within the chamber, a sample holder that can be manipulated to bring the crystal to any orientation with respect to the incident beam, and an electron spectrometer which can rotate about the crystal, thus varying the take-off angle of the electrons being analyzed. The surface traced out by the entrance axis of the spectrometer is coplanar with the incident

beam. This equipment is housed in a stainless-steel chamber, with a pressure of less than 2.5×10^{-11} Torr, a magnetic field less than 2 mG, and a low, but unknown, electric field. For the data presented the angular resolution is about 1.25° , and the energy resolution 0.1 eV.³

The silicon crystal used was cut from a 4- Ω -cm *n*-type wafer. This sample was chemically cleaned in the manner described by Chang,⁴ mounted in tantalum slips, and cleaned in the vacuum by heating to 870°C for about an hour.⁴ The surface thus prepared gave a distinct (111)-7 × 7 elastic-low-energy-electron-diffraction (ELEED) pattern, as measured by angular scans of the elastic peak in the $[2\bar{1}\bar{1}]$ and $[1\bar{1}\bar{2}]$ azimuths.

For fixed incident-beam conditions the energy spectrum was measured at each of a series of angles of emergence. The zero of kinetic energy was determined from the threshold of the spectrum of electrons emerging along the surface normal, in the usual manner.^{1,2}

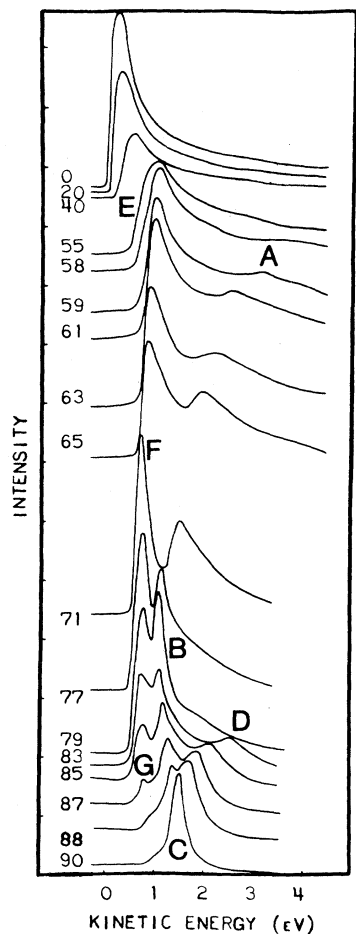


FIG. 1. Secondary-electron-emission spectra from a Si(111)7 \times 7 surface. The number to the left of each spectrum is the angle of emergence, in degrees, from the surface normal. The intensities of the spectra from 0 $^\circ$, 20 $^\circ$, and 40 $^\circ$ have been reduced by a factor of 3.

The spectra shown in Fig. 1. were recorded for an 80-eV exciting beam incident at $20 \pm 1^\circ$ azimuth. The angles of emergence for all the spectra discussed here lie in the $[2\bar{1}\bar{1}]$ azimuth. The $[\bar{2}11]$ and $[2\bar{1}\bar{1}]$ azimuths are coplanar, lying on opposite sides of the surface normal, $[111]$.

For normal emergence (0 $^\circ$ in Fig. 1), the intensity in the spectrum is a maximum at the threshold. With increasing angle of emergence the threshold moves to higher energy.³ At about 60 $^\circ$ from the normal the peaks labeled A and E appear. These peaks clearly belong to two series of peaks which are observed for even larger angles of emergence: The series starting at A moves first towards lower energies to B, then out to C. The other series of peaks starts at E, moves with notable increase of intensity to F,

and then out to G. Past G this series appears as a shoulder on the low-energy side of peaks in the series B-C. Another series of peaks, starting with D, is also apparently related to the peak at C.

No sign of these peaks is observed in EADSEE from a silicon (111)1 \times 1, unreconstructed surface, for a variety of input-beam conditions: The peaks have their origin in the reconstructed-surface layer. The 1 \times 1 surface was prepared by heating to 1050 $^\circ$ C for several minutes. This treatment brings small amounts of impurities to the surface,⁴ although probably not sufficient to contribute appreciably to electron scattering.⁵ The EADSEE from the 1 \times 1 surface exhibited structure at higher energies which could be associated with bulk band structure.^{2,3}

The peaks in the spectra of Fig. 1 are interpreted as arising from a two-step process: Valence electrons are excited into surface states which lie above the vacuum level, subsequently leaking out into the vacuum to be detected as secondary electrons. This two-step process is the surface analog of the three-step process, excitation, transport, and emergence, normally used to describe secondary emission from bulk conduction states.⁶ As shown later, the other surface-related explanation of the peaks cannot describe all of the data.

For electrons crossing an ordered surface into the vacuum energy is conserved, and

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

where k_{\parallel} is the component of the electron wave vector parallel to the surface, and b_{\parallel} is a surface reciprocal-lattice vector. Thus electrons from a state with energy ϵ above the vacuum level, and wave vector k_{\parallel} , will give rise to a peak in the EADSEE at energy ϵ and angle θ , where $k_{\parallel \text{out}}$ is measured as $\epsilon^{1/2} \sin \theta$. On this model the dispersion curve, ϵ versus k_{\parallel} , for the series of peaks of Fig. 1, should resemble that for surface states. A comparison between the two is made below.

In Fig. 2 is a plot of ϵ versus k_{\parallel} for the peaks. It includes points from six runs. Parts of the curve identified with letters correspond to peaks in the spectra similarly labeled. Points corresponding to the series of shoulders on the continuation of the series E-F-G in Fig. 1 are shown as open circles in Fig. 2. Their location has larger uncertainties than others. In Fig. 2 the values of $k_{\parallel} + b_{\parallel}$ for $k_{\parallel} = 0$ and for the zone boundary are indicated. The point $K = 0$ corresponds

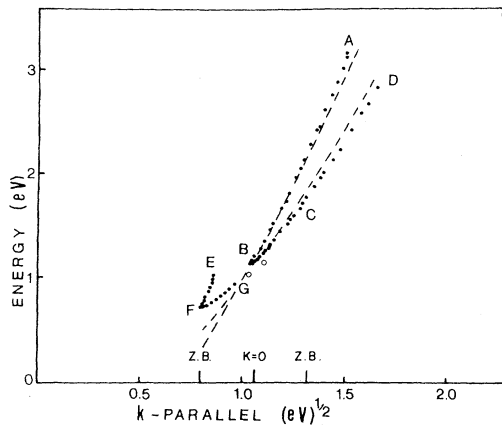


FIG. 2. Dispersion curves: dots for the peaks in Fig. 1; dashed lines for free electrons.

to twice the 7×7 surface reciprocal-lattice vector. Within experimental error, points C and F have wave vectors at the zone boundary and point B is at the center of the zone to within an integral number of surface reciprocal-lattice vectors.

There is no calculation with which these results can be directly compared, although related calculations are available.⁷ A general theory for surface-state resonances has been presented by McRae.⁸ To lowest order, in a nearly-free-electron model, the energy of a state with k_{\parallel} can be expanded about reciprocal-lattice points as⁸

$$E(k_{\parallel}) = K_v^2 + (M_1 a_1 + M_2 a_2 + k_{\parallel})^2,$$

where a_1 and a_2 are the basic surface reciprocal-lattice vectors, the M 's are integers, and K_v is a constant.

The nearly-free-electron dispersion curves along the direction lying in the $[2\bar{1}\bar{1}]$ azimuth have been calculated for energies up to 7 eV above the bottom of the band ($M_1 = M_2 = k_{\parallel} = 0$). The part of the calculated dispersion curve that best fits the experimental data is shown in Fig. 2 by dashed lines. The energy of the curve has been adjusted to fit the experimental point at B. In terms of basic reciprocal-lattice vectors point B has components (3, 1) and (1, 3) and lies 3.64 eV above the bottom of the band. The agreement in the region A-B-D is quite good. However, there are departures from free-electron behavior so that the particular assignment is not unique. It is the general agreement between the forms of the two dispersion curves that supports the model.

The most radical departure from free-electron behavior comes in the branch E-F (Fig. 2). In

the model there is no branch point anywhere on the zone boundary. Peak E appears to be connected to both the bulk and the surface states as it has ϵ and k_{\parallel} which overlap with those of bulk states which give rise to emission at 59° , and is the first member of the series of peaks which are associated with the reconstructed surface. The origin of peaks E to F might be related to the fact that they appear at values of ϵ and k_{\parallel} near the limit of stability for these surface-state resonances, i.e., near the region where matching with bulk states is possible.⁸ However, the explanation of these peaks, as well as a theoretical investigation of the specific origin of all the states, is left to others. It is noted that the shapes and energies of peaks E to F were the features most sensitive to variations of heat treatment, and to the time between that treatment and measurement.

The interpretation in terms of emission from surface states gets some support from the work of Rowe and Ibach,⁹ who measured the spectra of electrons inelastically scattered from a silicon (111) 7×7 surface. They observed a surface energy-loss peak at 7.4 ± 0.4 eV, associating it with an electronic transition to higher-energy surface states from either a state about 6 eV below the top of the valence band or states near the top of the valence band. On the basis of the known ionization energy of electrons at this surface, 5.0 ± 0.1 eV,¹⁰ these higher-energy states would lie 2.4 ± 0.4 eV above the vacuum level, which is within the energy region of the states observed here (Fig. 1).

In the spectra of Fig. 1 peak C appears unique, occurring at grazing emergence and having two series leading up to it. In Fig. 2, however, C seems to be just another point on the curve. States at C are simultaneously eigenstates of both the vacuum and of the crystal surface, with k_{\parallel} at the zone boundary.

A brief study of the dependence of these spectra on the energy of the exciting beam, at the same angle of incidence as for the data of Fig. 1, has been made. Identical peak structure was observed for incident energies of 32, 80, 100, and 120 eV. The intensity of the peaks, relative to the threshold feature at 0° , did vary considerably with incident energy. The peaks were absent for incident energies of 50 and 320 eV.³ Structure in EADSEE could be due to the modulation of the transmission probability for electrons crossing the surface layer in going from bulk conduction states to the vacuum. In this case the intensity

of the peaks, relative to the intensity of the threshold feature at 0° emergence, would be relatively insensitive to excitation energy. This behavior was not observed for the peaks in the spectra of Fig. 1.

In summary, the evidence associating the secondary-emission peaks with states in the reconstructed-surface layer is substantial: viz., the comparison of EADSEE from two different silicon (111) surfaces, turning points in the dispersion curves having values of k_{\parallel} that have significance for the reconstructed surface, but not for the bulk, and the agreement between the forms of the observed and calculated dispersion curves. The specific mechanism put forward, that of emission from surface states, rather than tunneling through them, is strongly supported by the excitation data.

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Bound Trinucleon System Using a One-Boson-Exchange Potential*

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The relativistic one-boson-exchange potential of Holinde, Erkelenz, and Alzetta is used to calculate the ^3He binding energy (E_3), wave function, and charge form factor. The calculation uses the 1S_0 and $^3(S-D)_1$ two-nucleon states and all the three-nucleon states that can then occur. The binding energy was found to be 6.75 MeV; the wave function composition was $P(S)=92.8$, $P(S')=1.6$, and $P(D)=5.7$; and the form factor had a diffraction minimum at $Q^2=16.8 \text{ fm}^{-2}$ and a secondary maximum of strength 5.8×10^{-4} at $Q^2=22.8 \text{ fm}^{-2}$.

Recently Holinde, Erkelenz, and Alzetta¹ have reported a representation of the nucleon-nucleon two-body force which reproduces the $N-N$ data with about as good an accuracy as does the best phenomenological potential, e.g., Reid's soft-core potential (RSC).² It has the additional practical advantage that it is derived naturally in momentum space,³ thus making it convenient for Faddeev calculations via the two-body Lippmann-Schwinger equation. It is a somewhat more fundamental description of the $N-N$ interaction, derived as it is from relativistically invariant Lagrangians and containing off-shell behavior based on covariant perturbation theory. An excellent description of the potential and of one-boson-exchange potentials (OBEP) in general is contained in the review article by Erkelenz.⁴

The particular version of the potential used in this report is that referred to as OBEP(I).⁵ It contains the effects of exchange of the mesons π ($J^\pi=0^-, I=1$), η ($J^\pi=0^-, I=0$), δ ($J^\pi=0^+, I=1$), σ ($J^\pi=0^+, I=0$), ρ ($J^\pi=1^-, I=1$), ω ($J^\pi=1^-, I=0$), and φ ($J^\pi=1^-, I=0$), where the quantum numbers in parentheses have their usual meaning.