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Photoemission study of the surface and bulk electronic structures of Si(111)7$\times$7 and Si(111)$\sqrt{3}\times\sqrt{3}$:Al

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Angle-resolved photoelectron spectroscopy has been used to study the surface and bulk electronic structures of Si(111)7$\times$7 and Si(111)$\sqrt{3}\times\sqrt{3}$:Al. For the Si(111)7$\times$7 surface we find three surface states at ≈ -0.2 (S_1), ≈ -0.8 (S_2), and ≈ -1.8 (S_3) eV. The S_3 surface state shows dispersion along the $\overline{\Gamma}$–$\overline{K}$ and $\overline{\Gamma}$–$\overline{M}$ lines in the 1$\times$1 surface Brillouin zone, with a bandwidth of $\approx$0.3 eV. For Si(111)$\sqrt{3}\times\sqrt{3}$:Al we find two surface-state structures A_1 and A_3 which are similar to the S_1 and S_3 structures for the 7$\times$7 surface. Structures due to direct transitions from the uppermost two valence bands are also identified in the spectra. Initial energy versus wave vector parallel to the surface, $E_i(\bar{k}_{\|})$, dispersions are presented along the [11$\bar{2}$], [2$\bar{1}\bar{1}$], and [10$\bar{1}$] azimuthal directions. The experimental dispersions for the direct transitions are in good agreement with calculated dispersions using a free-electron final band.

I. INTRODUCTION

The atomic and electronic structures of reconstructed semiconductor surfaces have been the object of many theoretical and experimental studies. Among the more complex reconstructed semiconductor surfaces, Si(111)7$\times$7 is the most studied. Due to its large unit cell it has not been possible to calculate the electronic structure of this surface. A detailed comparison with angle-resolved photoemission results thus cannot at present be made.

Experimentally it is well established that the photoemission spectra of the Si(111)7$\times$7 surface exhibit three surface-state peaks at ≈ -0.2, ≈ -0.8, and ≈ -1.8 eV relative to the Fermi level[1] (E_F) (denoted by S_1, S_2, and S_3, respectively, in Fig. 1). In the present work we report an initial-energy dispersion for the S_3 surface state along the $\overline{\Gamma}$–$\overline{K}$ and $\overline{\Gamma}$–$\overline{M}$ symmetry lines in the 1$\times$1 surface Brillouin zone (SBZ), with a bandwidth of $\approx$0.3 eV. A measurable dispersion along $\overline{\Gamma}$–$\overline{M}$ close to $\overline{M}$ was reported earlier by Neddermeyer *et al.*[2]

In an earlier work,[3] the S_3 surface state was deduced to have Λ_3 symmetry from the increase in emission intensity at ≈ -2 eV in normal emission for *s*-polarized light. This symmetry assignment is questioned here since the peak at ≈ -2 eV is shown in the present paper to be due to direct transitions from the Λ_3 valence band. For off-normal emission the emission intensity dependence of S_3 on the angle of light incidence is the same as for a dangling-bond state, indicating that S_3 could be dangling-bond derived instead of back-bond derived, as is often assumed.

We have also studied the electronic structure of the Si(111)$\sqrt{3}\times\sqrt{3}$:Al surface which is found to have similar electronic structure to Si(111)7$\times$7. The main difference is that the ≈ -0.8-eV state is absent for the $\sqrt{3}\times\sqrt{3}$ surface, while we find two surface states qualitatively similar to the S_3 and S_1 surface states of the 7$\times$7 surface. The dispersion of the lower surface state of the $\sqrt{3}\times\sqrt{3}$:Al surface has been reported by Hansson *et al.*,[4] along the $\overline{\Gamma}$–$\overline{M}'$ and $\overline{\Gamma}$–$\overline{K}'$–$\overline{M}'$ directions of the $\sqrt{3}\times\sqrt{3}$ SBZ. Along these two directions they found different energies for the $\overline{M}'$ points, which is not consistent with a single band having the $\sqrt{3}\times\sqrt{3}$ periodicity. From theoretical considerations, they predicted the existence of two filled surface-state bands, which could possibly account for the two different $\overline{M}'$ energies. Our results confirm their experimental finding of different $\overline{M}'$ energies. We have not found any further evidence for two surface bands which could explain the problem of different $\overline{M}'$ energies. Instead, we find that the dispersion follows the 1$\times$1 SBZ symmetry.

Proceeding from the 7$\times$7 to the $\sqrt{3}\times\sqrt{3}$ reconstruction, an interesting change occurs in the emission from the bulk bands. The broad emission peaks from the bulk bands for Si(111)7$\times$7 become sharp for the $\sqrt{3}\times\sqrt{3}$ surface, and we can positively identify structures corresponding to direct transitions from the uppermost two valence bands. The initial-energy dispersions as a function of wave vectors parallel to the surface, $E_i(\bar{k}_{\|})$, are presented along the [11$\bar{2}$], [2$\bar{1}\bar{1}$], and [10$\bar{1}$] directions, and they are found to be in good agreement with calculated dispersions obtained with the use of a free-electron final-state band.[5,6]

II. EXPERIMENTAL DETAILS

The photoemission experiments were performed in a VG ADES 400 UHV spectrometer (base pressure $\approx 1\times10^{-10}$ Torr), equipped with angle-resolved ultraviolet photoelectron spectroscopy (ARUPS), x-ray photoelectron spectroscopy (XPS), and low-energy electron diffraction (LEED) facilities. The total-energy resolution was $\leq$0.2 eV in the spectra, obtained here using unpolar-

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ized HeI resonance light. The sample was a Si(111) single crystal of p type ($\rho \approx 5000$ Ω cm), with a size of $12 \times 12 \times 0.2$ mm^3, cut from a wafer. To check the crystal orientation the Laue method was used. Repeated cycles of Ar$^+$ sputtering and annealing ($\approx 800\,^\circ$C, 5 min) resulted in a sharp 7×7 LEED pattern.

The well-ordered Si(111)$\sqrt{3} \times \sqrt{3}$:Al surfaces were obtained by evaporating ≈ 2 monolayers (ML) of Al, as monitored by a quartz-crystal microbalance, onto the Si(111)7×7 surface and then annealing at $850\,^\circ$C for 30 sec. After annealing the amount of Al was consistent with a $\frac{1}{3}$ ML coverage[4] as monitored by the intensity of the Al $2p$ peak in XPS. Annealing at lower temperatures resulted in the coexistence of $\sqrt{7} \times \sqrt{7}$ and $\sqrt{3} \times \sqrt{3}$ domains, and annealing at higher temperatures resulted in 7×7 domains. The LEED patterns from the $\sqrt{3} \times \sqrt{3}$ surfaces were very sharp, comparable to those observed from the best cleaved 2×1 surfaces. By annealing at $\approx 1000\,^\circ$C for 5 min or by sputtering and annealing, the 7×7 reconstruction could be regained. These two procedures resulted in identical ARUPS spectra for Si(111)7×7.

III. EXPERIMENTAL RESULTS

A. Si(111)7×7

Photoemission spectra from Si(111)7×7 obtained at a photon energy of 21.2 eV are shown in Fig. 1 for various angles of emission (θ_e). The azimuthal orientation of the sample is such that off-normal emission probes the $\bar{\Gamma}-\bar{K}$ line in the 1×1 SBZ (see Fig. 2). The S_1 and S_2 surface states are observed at ≈ -0.2 and ≈ -0.8 eV, respectively. The maximum in emission intensity for the S_1 peak was observed at around $\theta_e = 10^\circ$ in both the $\bar{\Gamma}-\bar{K}$ and $\bar{\Gamma}-\bar{M}$ directions, in agreement with earlier experimental results.[2,7,8] The S_2 surface state is observed in the whole 1×1 SBZ with approximately constant emission intensity. No $E_i(\bar{k}_{\parallel})$ dispersion was observed for the S_1 and S_2 surface-state structures.

The third surface state S_3 is the dominant structure at -1.75 eV for $\theta_e = 20^\circ$. It disperses downwards for higher emission angles. The total bandwidth is ≈ 0.3 eV. For smaller emission angles the intensity decreases and it is difficult to identify the S_3 surface-state structure. The dispersion along the $\bar{\Gamma}-\bar{K}$ line is plotted as open circles in Fig. 3, which also includes the upper limit of the projected bulk bands from Ref. 9. We have used $E_F - E_V = 0.59$ eV for Si(111)7×7.[10] Note that in the $\bar{k}_{\parallel}$ range of high emission intensity, the S_3 initial energies lie in the projected bulk band gap. The dispersion along $\bar{\Gamma}-\bar{M}$ is shown in Fig. 4.

The symmetry of the S_3 surface state has earlier been reported from measurements in normal emission using polarized light ($\hbar\omega = 21.2$ eV).[3] Due to an increase in the emission intensity of the ≈ -2-eV peak for s-polarized light, the authors deduced that S_3 has Λ_3 symmetry. In the present experiment we find that the ≈ -2-eV peak in normal emission corresponds to a direct transition from the uppermost Λ_3 bulk band, and thus we find that no unambiguous symmetry assignment of the S_3 surface state can be made at $\hbar\omega = 21.2$ eV. The direct transition giving rise to the ≈ -2-eV peak will be discussed in more detail below for the Si(111)$\sqrt{3} \times \sqrt{3}$:Al case. At a photon energy of 52 eV, Houzay *et al.*[11] reported a structure of

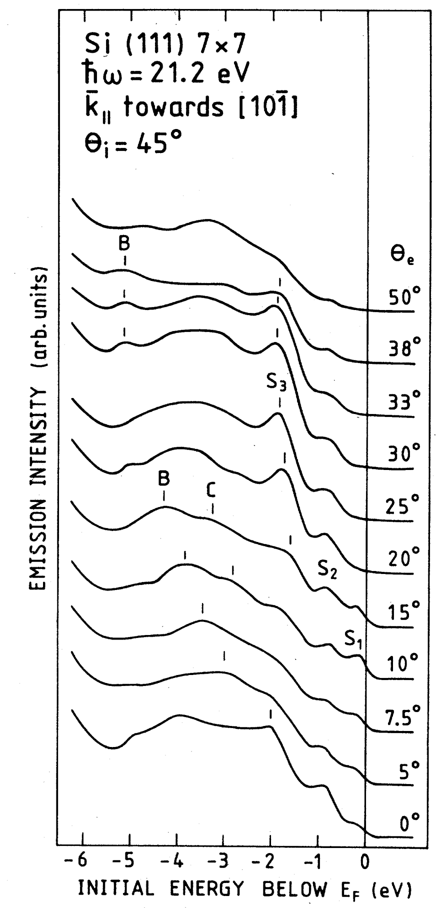

FIG. 1. Photoemission spectra for various angles of emission (θ_e). Structures S_1, S_2, and S_3 correspond to surface-state emission. Structures B and C are due to direct bulk transitions.

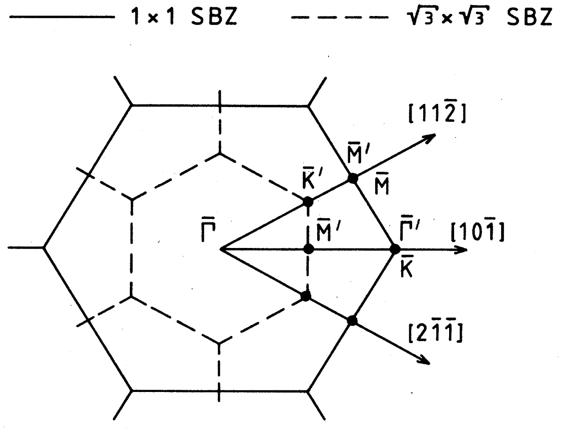

FIG. 2. Directions probed in the 1×1 and $\sqrt{3} \times \sqrt{3}$ surface Brillouin zones. Symmetry points are indicated.

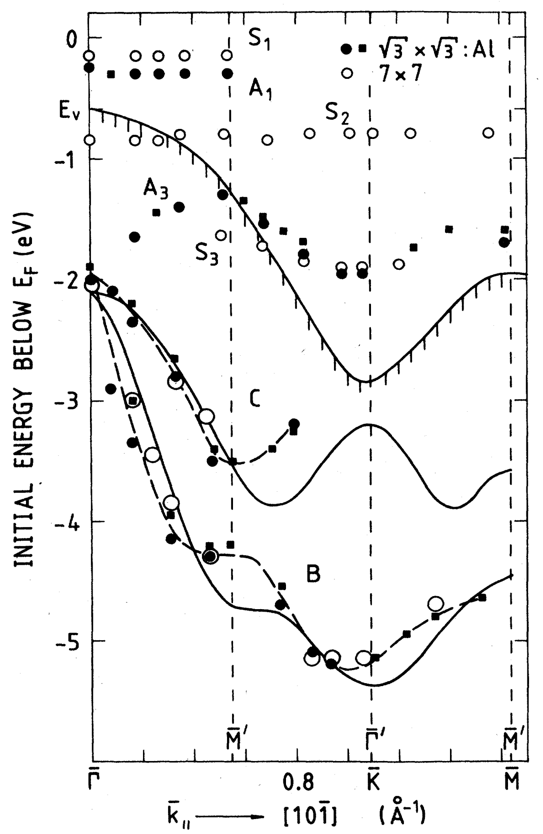

FIG. 3. Experimental initial-energy versus $\bar{k}_{\|}$ plots for different surface and bulk structures for Si(111)7×7 (open circles) and for Si(111)$\sqrt{3}\times\sqrt{3}$:Al (solid circles and squares). Solid curves show calculated dispersions for the direct transitions *B* and *C*. Also included is the top of the projected bulk bands from Ref. 9.

Λ_3 symmetry at -1.8 eV in normal emission, which they interpreted as the S_3 surface state. Since one cannot definitely show that the -1.8-eV structure at $\hbar\omega=52$ eV has the same origin as the dispersing S_3 band at $\hbar\omega=21.2$ eV, we find that the symmetry of the S_3 surface state is still an open question.

For off-normal emission in which S_3 can be unambiguously identified, the dependence of emission intensity of S_3 on the angle of light incidence is the same as for a dangling-bond surface state. For a decreasing component of the electric field vector perpendicular to the surface (E_z), the emission intensity decreases. This is shown in Fig. 5 for $\theta_e=25°$, where the S_3 peak is smaller for $\theta_i=15°$ (E_z small) than for $\theta_i=45°$.

The sensitivity of structures S_2 and S_3 to oxygen exposure is shown in Fig. 6 for exposures between 0 and 2 L (1 L$\equiv 1\times10^{-6}$ Torr s). Emission from the surface states is highly reduced for an exposure of 2 L. At this exposure a 7×7 pattern is still observed in LEED, but with an increased background. The adsorbed oxygen results in additional intensity at ≈ -7 eV in the spectra for the 1- and 2-L exposures. The structure at ≈ -7.5 eV for the clean surface corresponds to bulk emission from silicon.

In a gas-exposure experiment performed at 10.2 eV, a significant difference in the effect of oxygen and chlorine exposures was observed. In the initial stage of oxygen exposure structure S_1 is the first to disappear, while S_2 is still observed. For chlorine exposures the relative sensitivity of structures S_1 and S_2 was found to be the opposite to that for oxygen. This is shown in Fig. 7 where the S_2 surface state is still observed after a moderate oxygen exposure, while after the chlorine exposure the S_1 surface state is still observed. There is a gradual downward shift of the S_1 peak ≤ 0.15 eV relative to both E_F and the bulk contributions for increasing chlorine exposures. It thus seems that the S_1 surface state is only modified by the

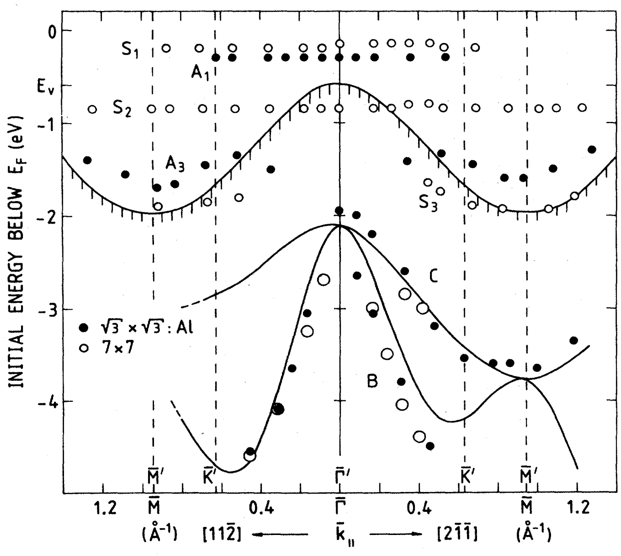

FIG. 4. Initial-energy versus $\bar{k}_{\|}$ relations as in Fig. 3, but for different azimuthal directions.

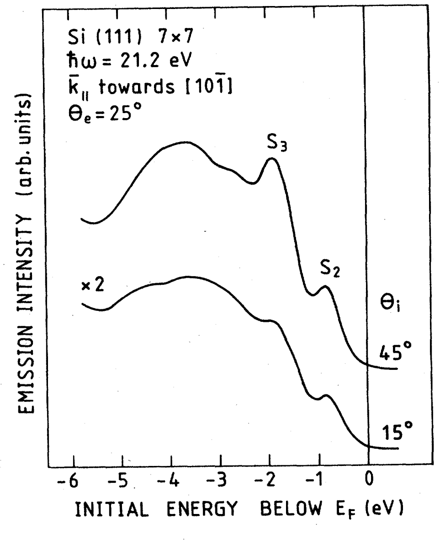

FIG. 5. Dependence of the S_2 and S_3 surface-state emission on the angle of light incidence.

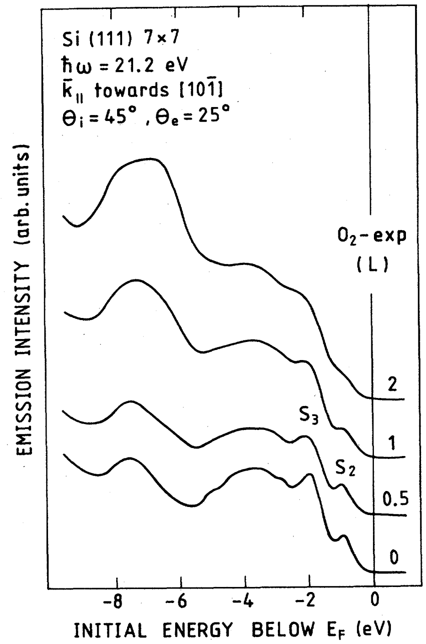

FIG. 6. Effect of oxygen exposure on the S_2 and S_3 surface-state emission.

presence of chlorine, while the S_2 surface state disappears. In the initial-energy range from -2 to -5 eV, we find some broad structures (B and C in Fig. 1) dispersing downwards for increasing emission angles. These structures are due to direct transitions from the uppermost two valence bands. The $E_i(\bar{k}_{\parallel})$ dispersions are in good agreement with calculated dispersions for direct transitions to a free-electron final band.[5,6] The experimental dispersions are plotted as open circles in Fig. 3 and 4. These direct transitions will be further discussed below for the Si(111)$\sqrt{3}\times\sqrt{3}$:Al case.

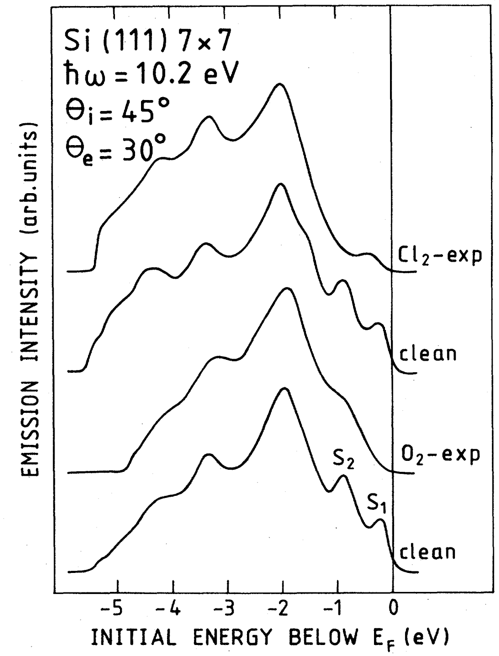

FIG. 7. Effect of oxygen and chlorine exposure on the S_1 and S_2 surface-state emission.

B. Si(111)$\sqrt{3}\times\sqrt{3}$:Al

Spectra for different emission angles are shown in Fig. 8 for the [10$\bar{1}$] azimuthal direction. The symmetry lines probed in the SBZ's are shown in Fig. 2. For the $\sqrt{3}\times\sqrt{3}$:Al surface, we observe two surface-state structures A_1 and A_3, which are similar to the S_1 and S_3 surface states on the Si(111)7×7 surface. The A_1 structure is found at ≈ -0.3 eV and it has maximum intensity for $\theta_e \approx 10°$, which is in close agreement with the behavior found for S_1. Compared with S_3, the A_3 surface state has higher emission intensity and a larger bandwidth (≈ 0.65 eV), but the dispersion is qualitatively similar to that found for structure S_3. The dispersion of structure A_3 along the [10$\bar{1}$] direction from two $\sqrt{3}\times\sqrt{3}$ surfaces (solid circles and squares) is shown in Fig. 3, and along the [11$\bar{2}$] and [2$\bar{1}\bar{1}$] directions in Fig. 4. Indicated in Figs. 3 and 4 are the symmetry points for the $\sqrt{3}\times\sqrt{3}$ and 1×1 SBZ's from Fig. 2. Our experimentally found dispersions are in agreement with those presented in Ref. 4, although we find a 0.25 eV larger bandwidth. In accordance with this earlier study we find different initial ener-

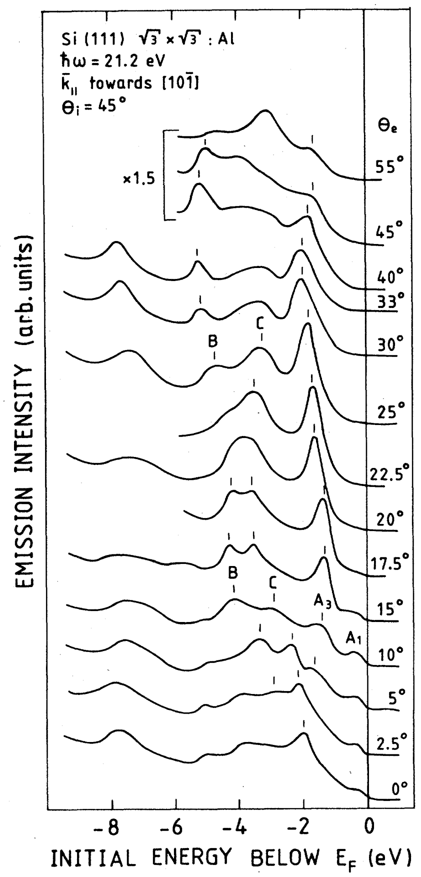

FIG. 8. Photoemission spectra for various angles of emission (θ_e). A_1 and A_3 correspond to surface-state emission. Structures B and C are due to direct bulk transitions.

gies for the A_3 surface state at the two $\bar{M}'$ points along the $\bar{\Gamma}-\bar{M}'$ and $\bar{\Gamma}-\bar{K}'-\bar{M}'$ lines of the $\sqrt{3}\times\sqrt{3}$ SBZ. As seen from Figs. 3 and 4, the $\bar{M}'$-point energies are -1.3 eV and ≈ -1.6 eV, respectively. In Ref. 4 the different $\bar{M}'$-point energies were taken as experimental evidence for two occupied surface-state bands, although only a single peak was observed in the spectra. The A_3 peaks obtained at the two $\bar{M}'$ points are shown in Fig. 9. The lower spectrum was obtained in the $\bar{\Gamma}-\bar{M}'$ direction and the upper two spectra in the $\bar{\Gamma}-\bar{K}'-\bar{M}'$ direction. If there were two filled bands we would expect to have an additional structure in the uppermost two spectra at the initial energy of the A_3 peak in the lowest spectrum (position of the dashed line). We have not been able to detect any such additional structure, and since we have used unpolarized light incident at 45°, we do not expect that the emission intensity from one of the suggested bands should be selectively reduced. We find that the dispersion of the A_3 surface state is consistent with the 1×1 SBZ, having the same initial energy for the two $\bar{M}$ points of the 1×1 SBZ. Like S_3, the A_3 surface state is excited by the E_z component of the incidence light.

The broad bulk structures observed for Si(111)7×7 correspond to much sharper structures in the $\sqrt{3}\times\sqrt{3}$ case. In Fig. 8 one clearly sees that the ≈ -2-eV peak for $\theta_e=0°$ disperses downwards for increasing emission angles (C), and hence should not be confused with the A_3 or S_3 surface states. The experimental $E_i(\bar{k}_{\parallel})$ dispersions of the bulk structures B and C are plotted in Fig. 3 along the $[10\bar{1}]$ direction and in Fig. 4 along the $[11\bar{2}]$ and $[2\bar{1}\bar{1}]$ directions. The solid curves are the calculated $E_i(\bar{k}_{\parallel})$ dispersions for direct transitions from the uppermost two valence bands to the $\bar{k}+\bar{G}_{111}$ free-electron final band. The application of the $\bar{k}+\bar{G}_{111}$ free-electron band as the final band has been discussed elsewhere.[5,6] In these earlier papers we obtained an experimental final band in normal emission from Si(111)2×1, which had a free-electron-like dispersion. To be able to calculate the $E_i(\bar{k}_{\parallel})$ dispersions for direct transitions this experimental final band was approximated by the $\bar{k}+\bar{G}_{111}$ free-electron band. Furthermore, the L_3' point in the valence bands was experimentally found at -1.6 eV, relative to the valence-band maximum, while the calculated L_3'-point energy is ≈ -1.2 eV.[5,6] When calculating the $E_i(\bar{k}_{\parallel})$ dispersions for direct transitions, we have therefore used valence bands which were lowered with respect to the calculated valence bands by an amount proportional to the distance from Γ so that the L_3'-point energy becomes -1.6 eV. The procedure described above is also applied in the present paper.

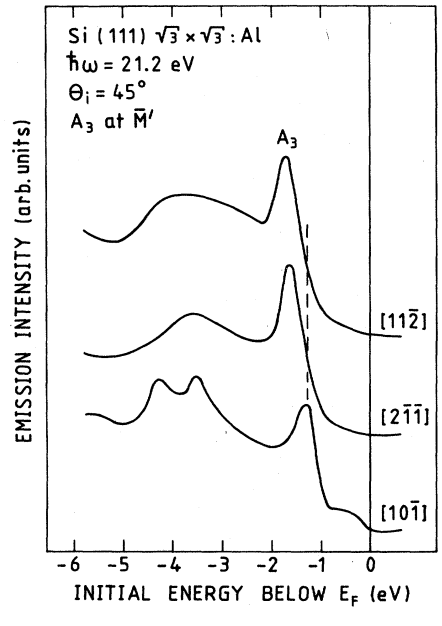

FIG. 9. A_3 surface state probed at different $\bar{M}'$ points in the $\sqrt{3}\times\sqrt{3}$ SBZ in the $\bar{\Gamma}-\bar{M}'$ direction (bottom spectrum), and in the $\bar{\Gamma}-\bar{K}'-\bar{M}'$ direction (uppermost two spectra). In the case of two occupied surface-state bands in the $\sqrt{3}\times\sqrt{3}$ SBZ one would expect a contribution in the two upper spectra at the position of the dashed line.

As can be seen from Figs. 3 and 4, there is good agreement between experimental and calculated $E_i(\bar{k}_{\parallel})$ dispersions for the direct bulk transitions B and C. The qualitative features of the experimental dispersions are well reproduced by the calculated dispersions as are the energy positions. The E_F-E_V value for the $\sqrt{3}\times\sqrt{3}$:Al surface is 0.05–0.10 eV smaller than for 7×7, as estimated from the energy position of the bulk structure at ≈ -2 eV. This means that in principle there should be another set of projected bulk bands and calculated dispersion relations for the $\sqrt{3}\times\sqrt{3}$ surface in Figs. 3 and 4, shifted by 0.05–0.10 eV upwards. We have omitted this in the figures due to the small energy shifts. From the results in this work and in Refs. 5 and 6, we can conclude that the $\bar{k}+\bar{G}_{111}$ free-electron band is a good approximation to the true final band, giving $E_i(\bar{k}_{\parallel})$ dispersions in good agreement with experiments in the photon energy range 10.2–21.2 eV investigated.

IV. DISCUSSION

For Si(111)7×7, we have found that the S_3 surface structure has dispersion in the 1×1 SBZ, with a bandwidth of ≈ 0.3 eV. The Λ_3 symmetry of this surface structure determined earlier from normal emission at $\hbar\omega=21.2$ eV (Ref. 3) is strongly questionable due to the interference of a bulk structure originating from direct transitions from the Λ_3 valence band. Instead, we find that the polarization dependence of structure S_3 for off-normal emission is consistent with a dangling-bond interpretation. The possibility then exists that the Si(111)7×7 surface has three dangling-bond surface states S_1, S_2, and S_3. A reconstruction model of the 7×7 surface would then have to explain the existence of three different dangling-bond-derived surface states.

Oxygen and chlorine exposures of the Si(111)7×7 surface resulted in different effects on the S_1 and S_2 surface-state emission. A moderate oxygen exposure removed the S_1 surface peak, while a chlorine exposure removed the S_2 surface peak (see Fig. 7). The difference in how the S_1 and S_2 surface-state peaks were affected by oxygen and chlorine indicates different adsorption sites for the two gases in the initial stage of exposure. Howeer, at present the specific adsorption sites cannot be determined since the dangling-bond positions to be associated with S_1 and S_2 depend on the atomic arrangement on the 7×7 surface, which is not sufficiently known.

It is interesting to note that the S_2 surface state, removed by chlorine, is not present on the $\sqrt{3}\times\sqrt{3}$:Al surface, which indicates that the sites involved in chlorine adsorption on 7×7 are missing on the $\sqrt{3}\times\sqrt{3}$:Al surface. On the other hand, S_1 and S_3 seem to have their counterparts in structures A_1 and A_3 on the $\sqrt{3}\times\sqrt{3}$:Al surface. The A_1 and A_3 surface states are, however, slightly altered compared to S_1 and S_3. The A_1 peak is shifted downwards ≈0.1 eV compared to S_1, while for A_3 we find a higher emission intensity and a ≈0.35 eV larger bandwidth than observed for S_3.

The experimental finding in Ref. 4; that the initial energy of structure A_3 is not the same at $\overline{M}'$ on the $\overline{\Gamma}-\overline{M}'$ and $\overline{\Gamma}-\overline{K}'-\overline{M}'$ lines, and that therefore the $E_i(\overline{k}_{\parallel})$ dispersion is not consistent with the $\sqrt{3}\times\sqrt{3}$ SBZ, is confirmed in the present study. Recently, Yokotsuka *et al.*[12] presented ARUPS data for Si(111)$\sqrt{3}\times\sqrt{3}$:Ag. They found two surface states at around -1 eV, one of which showed a dispersion consistent with a $\sqrt{3}\times\sqrt{3}$ SBZ. The experimental conditions in their measurements were similar to ours ($\hbar\omega=21.2$-eV unpolarized light and $\theta_i=45°$), but still for $\sqrt{3}\times\sqrt{3}$:Al the experimental dispersions are not related to a $\sqrt{3}\times\sqrt{3}$ SBZ.

In the initial-energy region -2 to -5 eV the dominating structures can be explained by direct transitions from the uppermost two valence bands to a free-electron band. The broadening of the bulk peaks for the 7×7 surface is attributed to scattering by the seventh-order reciprocal-lattice vectors. The direct transitions B and C can be identified in spectra obtained by other authors. For instance, in the $\theta_e=10°$ spectrum in Ref. 8, one can positively identify the structures at ≈-3 and ≈-4 eV as C and B. In Ref. 13 spectra for Si(111)2×1 along the $[10\overline{1}]$ direction obtained at 20.0 eV are presented. Since these spectra were obtained along the same azimuthal direction as the spectra presented in this paper and the photon energies are roughly the same, we can compare the spectra in the two studies. We find that the structure F at ≈-5 eV in Ref. 13 for Si(111)2×1 most likely corresponds to structure B for the 7×7 and $\sqrt{3}\times\sqrt{3}$ surfaces, and should not therefore be interpreted as a surface-state structure. Due to the large (10°) steps in emission angle in Ref. 13, it is difficult to make a positive identification of any structure corresponding to C.

To summarize, we find that the spectral features within 5 eV below E_F can be explained as surface states or bulk direct transitions for both Si(111)7×7 and Si(111)$\sqrt{3}\times\sqrt{3}$:Al. The dispersive surface states S_3 and A_3 have dispersions consistent with a 1×1 SBZ, instead of the expected 7×7 or $\sqrt{3}\times\sqrt{3}$ SBZ's, respectively. The free-electron final band introduced earlier[5,6] is found to give calculated $E_i(\overline{k}_{\parallel})$ dispersions in good agreement with experiments for transitions from the uppermost two valence bands.

Note added in proof. A recent calculation (Ref. 14) of the surface-state bands for Si(111)$\sqrt{3}\times\sqrt{3}$:Al shows two filled surface-state bands in the energy region where A_3 is found. The calculated bands are in good agreement with the experimental dispersion for A_3, when comparison is made in the 1×1 SBZ.

ACKNOWLEDGMENT

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