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Hanmin Zhang and Roger Uhrberg

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Ag/Si(111) $\sqrt{3}\times\sqrt{3}$: Surface band splitting and the inequivalent triangle model

H. M. Zhang^{*,†} and R. I. G. Uhrberg

Department of Physics, Chemistry and Biology, Linköping University, S-581 83 Linköping, Sweden

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The atomic and electronic structures of the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface are currently under debate. By employing angle-resolved valence-band spectroscopy, the surface band dispersions around the $\bar{K}$ point of the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface have been investigated in detail. Contrary to a recent study, we conclude that the S_2 and S_3 surface state bands do not show any detectable split at 100 K. Thus, photoemission spectra at both room temperature and 100 K show only a single peak at the $\bar{K}$ point without any direct evidence of a split. Calculated band structures for the inequivalent triangle (IET) model show a gap at the $\bar{K}$ point in contrast to the honeycomb-chain-trimer (HCT) model. We find, however, that there is no real contradiction between our photoemission data and the IET model provided the energy gap of the latter model is small as indicated by a recent calculation [Phys. Rev. B **70**, 245431 (2004)].

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As a prototypical system, the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface has been subjected to extensive studies during the past decades.¹ Low-temperature (LT) phase transitions and surface symmetry breaking are under current debate for this surface. The renewed interest in the surface atomic and electronic structure of Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ is partly based on a scanning tunneling microscopy (STM) observation.² At room temperature (RT), the STM image of the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface shows a honeycomb pattern, while at LT it exhibits a hexagonal pattern. An inequivalent triangle (IET) model³ was suggested for the ground state of the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ phase instead of the honeycomb-chain-trimer (HCT) model that has been widely used in the literature.⁴ The IET model was recently promoted by a LT (120 K) photoemission study that reported a surface band splitting and symmetry breaking on Ag/Si(111) $\sqrt{3}\times\sqrt{3}$.⁵ This result is, however, in contrast with earlier photoemission reports that no splitting was observed down to 70 K.^{6,7}

The Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface can be formed by annealing a Si(111) 7×7 surface covered by one monolayer (ML) of Ag atoms. In an earlier photoemission study,⁸ three surface-state bands (S_1 , S_2 , and S_3) were found along the $\bar{\Gamma}$ - $\bar{M}$ - $\bar{\Gamma}$ line of the $\sqrt{3}\times\sqrt{3}$ surface Brillouin zone (SBZ), while two surface bands (S_2' and S_3') were detected along the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ symmetry line. The metallic band (S_1) can be explained in terms of an adatom-induced partial occupation of an unoccupied band of the $\sqrt{3}\times\sqrt{3}$ surface.^{4,6-8} The other two surface bands, S_2' and S_3' , appeared to be degenerate at the $\bar{K}$ point and showed a polarization dependence consistent with an even and an odd symmetry with respect to a plane containing the surface normal and the $[11\bar{2}]$ direction. The symmetry properties have been regarded as a further support for the HCT model, for which this is a mirror plane.^{4,8} Recent studies have provided a more detailed picture of the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface. One observation is the presence of additional Ag atoms that are frozen into specific positions at temperatures below 62 K.⁹ When the extra Ag atoms are removed, the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface reveals its intrinsic electronic structure with well-resolved Si $2p$ core-level spec-

tra and two surface-state bands [S_2 (S_2') and S_3 (S_3')].⁷ Another interesting finding is the hexagonal pattern shown by LT STM images, which is in contrast with the honeycomb pattern observed at room temperature. An asymmetric appearance of protrusions in STM images has been interpreted as an atomic configuration change resulting in Ag trimers of two sizes.³ A transition from a surface described by the symmetric HCT model at RT to an asymmetric IET model was proposed to occur at low temperature. The transition temperature is believed to be somewhat below 150 K based on photoemission and x-ray diffraction measurements.^{5,10} The hexagonal appearance of the empty-state STM images and the IET model was supported by a theoretical calculation,³ which found that the IET model is more favorable, energetically, than the HCT model. As a consequence of the two different Ag trimers in the IET structure, the plane containing the surface normal and the $[11\bar{2}]$ direction is no longer a mirror plane. Due to the symmetry breaking, the S_2 and S_3 surface states, which are degenerate at the $\bar{K}$ point in the HCT model, were predicted to split in the IET model.^{2,3} In a recent angle-resolved photoemission study,⁵ the authors reported LT (120 K) spectra with a clear splitting of S_2 and S_3 at the $\bar{K}$ point of the $\sqrt{3}\times\sqrt{3}$ SBZ. In addition, their valence-band spectra did not show any specific symmetry for S_2 and S_3 in the plane containing the $[11\bar{2}]$ direction and the surface normal. Furthermore, the authors claimed that the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface exhibits a disorder-order phase transition, meaning that S_2 and S_3 are already split at room temperature at the $\bar{K}$ point.

In this paper, we present data from the Ag/Si(111) $\sqrt{3}\times\sqrt{3}$ surface obtained by angle-resolved photoelectron spectroscopy (ARPES). Low-energy electron diffraction (LEED) and core-level spectra were also used in order to optimize the sample preparation. Contrary to the recent study, we do not observe any splitting of the S_2 and S_3 surface-state bands at the $\bar{K}$ point of the $\sqrt{3}\times\sqrt{3}$ SBZ at 100 K. We demonstrate that an offset in the emission angle by 2.5° results in a splitting of S_2 and S_3 , similar to that reported in Ref. 5, for both the $A_{||}$ (A_+ in Ref. 5) and the $A_{\perp}$ (A_+ in Ref. 5) geometries.

FIG. 1. The geometry of the ARPES measurement. The sample is irradiated with photons with a polarization direction in the horizontal plane (xz plane). The emitted electrons can be detected in both the horizontal plane ($A_{||}$ geometry) and the vertical plane ($A_{\perp}$ geometry).

The photoemission study was performed at beam line 33 at the Max-I synchrotron radiation facility in Lund, Sweden. At this beam line, the degree of linear polarization is larger than 90% for energies less than 30 eV.¹¹ The angle-resolved valence-band spectra presented here were obtained with a total energy resolution of ~ 50 meV and an angular resolution of $\pm 2^\circ$. The Si(111) samples cut from a single-crystal wafer (Sb doped, $3 \Omega \text{ cm}$) were pre-oxidized by an etching method and cleaned *in situ* by stepwise direct current heating up to 930°C . This procedure resulted in a well-ordered surface, as evidenced by the strong surface-state emission and a sharp 7×7 LEED pattern. Ag was evaporated onto the Si sample from a tungsten filament source calibrated by a quartz crystal monitor. Evaporation of 1 ML of Ag followed by annealing at 530°C for 2 min resulted in a sharp $\sqrt{3} \times \sqrt{3}$ LEED pattern. The sample was then annealed at $\sim 600^\circ \text{C}$ for 1 min to remove extra Ag. To facilitate a comparison with earlier studies, all spectra presented here were recorded with a photon energy of 21.2 eV. The angle of the manipulator for normal light incidence was established by reflecting the synchrotron light back through the exit slit. The emission angle relative to the sample normal was calibrated by shining the zero-order light through the lens of the analyzer. Two measurement geometries have been used to investigate the polarization dependence of the surface-state emission. The electric-field vector was either in the plane defined by the surface normal and the $[11\bar{2}]$ direction or partially perpendicular to this plane depending on the incidence angle. These two cases are referred to as the $A_{||}$ case (horizontal angle scan) and the $A_{\perp}$ case (vertical angle scan), respectively. Figure 1 shows a schematic drawing of the measurement geometries. Compared to the early study that was done at RT,⁸ the current experiment was performed at both RT and 100 K with a full series of emission angles at each geometry. The Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface was better prepared by checking the S_1 surface state and the Si $2p$ core levels.⁷

Two sets of ARPES spectra from the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface along the $\bar{\Gamma}-\bar{K}-\bar{M}$ line of the $\sqrt{3} \times \sqrt{3}$ SBZ are shown in Figs. 2(a) and 2(b). These spectra were recorded in the $A_{\perp}$ geometry with two incidence angles (45° and 15°) at 100 K in the $[11\bar{2}]$ direction. In similarity with the earlier study, two surface-state bands are detected in this azimuthal direction.⁸ The spectra in Fig. 2(a) obtained with a 45° incidence angle

FIG. 2. ARPES spectra recorded from the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface with a photon energy of 21.2 eV at 100 K, along the $\bar{\Gamma}-\bar{K}-\bar{M}$ line of the $\sqrt{3} \times \sqrt{3}$ SBZ in the $A_{\perp}$ geometry (see inset). (a) with 45° incidence angle; (b) with 15° incidence angle; (c) with 45° incidence angle. The scan direction in (c) is perpendicular to the $\bar{\Gamma}-\bar{K}-\bar{M}$ line, crossing at the $\bar{K}$ point ($\theta_e = 18^\circ$, see inset).

show a strong surface state, S_2 , which is located at -1.1 eV at $\theta_e = 10^\circ$ and disperses downwards with increasing emission angle. S_2 reaches the $\bar{K}$ point of the $\sqrt{3} \times \sqrt{3}$ SBZ at $\theta_e = 18^\circ$. Beyond the $\bar{K}$ point, the single peak splits into two clear peaks. The stronger one disperses downwards to an initial energy of -1.45 eV at $\theta_e = 26^\circ$. The second surface state, S_3 , is very weak at low emission angles compared to S_2 . The spectra in Fig. 2(b), obtained with an incidence angle of 15° , show an intensity variation of S_2 and S_3 that is opposite to that in Fig. 2(a). The S_3 surface state is clearly detected at lower emission angles and it quickly disperses upwards. Beyond the $\bar{K}$ point, the peak splits in a way similar to that in Fig. 2(a), but in this case the upper peak is the stronger one. Thus the intensities of the two dispersive peaks in Figs. 2(a) and 2(b) are consistent with the original observation of the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface.⁸ However, to match the two $\bar{M}$ points along the $\bar{\Gamma}-\bar{K}-\bar{M}$ and $\bar{\Gamma}-\bar{M}-\bar{\Gamma}$ symmetry lines, one should assign the upper band as S_2 and the lower band as S_3 at $\theta_e = 26^\circ$ in Figs. 2(a) and 2(b), which is close to the $\bar{M}$ point.

To make sure that the spectra were recorded along the correct symmetry line, we used a different approach in this study. Instead of relying on the sample orientation determined by reflection high-energy electron diffraction⁵ or LEED, we have followed the dispersion of the surface-state bands themselves to find the correct angles for the $\bar{K}$ point. Figure 2(c) displays a set of spectra recorded with an incidence angle of 45° . The analyzer was set to a vertical emission angle of 18° (θ_v), and then the analyzer was scanned horizontally (θ_h). In a two-dimensional $\mathbf{k}$ space, this means a scan direction perpendicular to the $\bar{\Gamma}-\bar{K}-\bar{M}$ line at the $\bar{K}$ point

[see the inset in Fig. 2(c)]. Furthermore, it approaches the $\bar{\Gamma}$ - $\bar{M}$ - $\bar{\Gamma}$ line in the $\sqrt{3} \times \sqrt{3}$ SBZ. The S_2 and S_3 bands must be symmetric with respect to positive and negative angles in Fig. 2(c) since the experiment probes equivalent $\mathbf{k}$ points in this case. Thus the upper band in Fig. 2(c) should be S_2 , and the lower one should be S_3 . This is because the upper band is always S_2 along the $\bar{\Gamma}$ - $\bar{M}$ - $\bar{\Gamma}$ line.

The observation of a single peak at the $\bar{K}$ point in Fig. 2 is in sharp contrast to the recent photoemission study of the same surface, in which a splitting between S_2 and S_3 with a gap as large as 0.22 ± 0.07 eV was reported at a reduced sample temperature (120 K).⁵ Since the sample preparation method and measurement geometries in Ref. 5 were very similar to what we have used, it is important to find the reason for the discrepancy. Figure 2(a) in this paper and Fig. 2(b) in Ref. 5 show spectra obtained under similar experimental conditions, but the two sets of spectra are quite different. In Fig. 2(a), only one peak was detected at the $\bar{K}$ point of the $\sqrt{3} \times \sqrt{3}$ SBZ ($\theta_e = 18^\circ$). In Fig. 2(b) of Ref. 5 there are two peaks near $\theta_e = 18^\circ$ and the narrowest gap between the two peaks is found at $\theta_e = 20^\circ$, which is 2° off from the $\bar{K}$ point. As illustrated in Fig. 2(c), the single peak splits into two for a small deviation from the $\bar{K}$ point. The 19° and 19.5° spectra in Fig. 2(c) of Ref. 5 are very similar to the spectrum that is 2.5° off from the $\bar{K}$ point in Fig. 2(c) of this paper. Their 20° spectrum is close to the 3.5° off spectrum in our Fig. 2(c). Thus the spectra in Fig. 2 in Ref. 5 are not fully representative of the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line of the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface. The observation of a split of S_2 and S_3 finds a natural explanation in terms of an offset in the emission angle.

Even though the spectrum only presents a single peak at the $\bar{K}$ point ($\theta_e = 18^\circ$), one could suspect that the peak consists of two separate components. To obtain more detailed information, we have decomposed the spectra and made comparisons for various emission angles. Figure 3 shows such decomposed spectra obtained by a fitting procedure. An integrated background and Gaussian components with variable widths have been used. As shown in Fig. 3, all surface states in the spectra can be fitted with a Gaussian full width at half-maximum (FWHM) of ~ 0.24 – 0.29 eV. These values are smaller than those used in Ref. 5 (0.29 – 0.34 eV). In Fig. 3, one notices that the peak at $\theta_e = 18^\circ$ looks slightly broader than the peaks at $\theta_e = 10^\circ$ and 26° . The $\pm 2^\circ$ angular resolution results in a $\mathbf{k}$ resolution of ± 0.07 Å at $\theta_e = 18^\circ$. Since the two surface bands have strong dispersions near the $\bar{K}$ point, an uncertainty in the $\mathbf{k}$ vector around the $\bar{K}$ point naturally causes a slight broadening of the peak. To conclude this part, only one component is needed to fit the spectrum at $\theta_e = 18^\circ$, and therefore there is no direct spectral evidence of a surface band splitting at the $\bar{K}$ point at 100 K. This result once again confirms our earlier conclusion that was based on measurements down to 70 K.^{6,7}

We have also investigated the symmetry properties of the surface bands in the $A_{||}$ geometry. Figure 4 shows ARPES spectra from the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface recorded in the $A_{||}$ geometry with a 30° incidence angle at 100 K. As evidenced in Fig. 4(a), there is only one peak detected near the

FIG. 3. ARPES spectra recorded with a photon energy of 21.2 eV at emission angles of 10° , 18° , and 26° at 100 K [from Fig. 2(a)]. The two surface states in the spectra are fitted with Gaussian widths of ~ 0.24 eV at 10° and 26° emission angles. The spectrum at 18° emission angle is fitted with a Gaussian width of 0.29 eV. An integrated background has been used.

$\bar{K}$ point ($\theta_e = 17.5^\circ$). The S_2 surface state shows a strong intensity for $\theta_e = 11.5^\circ$, while the S_3 surface state is weak. Identifying the strongest peak in each spectrum as S_2 , one obtains a strong downward dispersion. Such identification implies that S_3 disperses upwards and that the two bands cross at the $\bar{K}$ point. Symmetry selection rules applied to the photoemission spectra in Figs. 2(a), 2(b), and 4(a) suggest that the S_2 band has an even symmetry and that the S_3 has a predominantly odd character with respect to the plane containing the surface normal and the $[11\bar{2}]$ direction. Such an identification of the surface bands and symmetry assignments was suggested in Ref. 8. In an ideal $A_{||}$ geometry, the S_3 surface state should not be observed along the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line, under perfect experimental conditions, if it has an odd symmetry. Several factors, such as the nonideal linear polarization ($< 100\%$) and the limited angular resolution of the analyzer ($\pm 2^\circ$), can explain a finite intensity of the S_3 surface state. However, a nonideal odd (even) character may also indicate a broken symmetry as predicted by the IET model. In such a case, the bands would not cross at the $\bar{K}$ point, but the split must be small enough to escape detection by photoemission.

In contrast to Fig. 4(a), quite different spectra, obtained with the same measurement geometry, were presented in Fig. 4 of Ref. 5. Those spectra show a clear split between S_2 and S_3 and a strong S_3 peak on both sides of the $\bar{K}$ point. To

FIG. 4. ARPES spectra recorded with a photon energy of 21.2 eV at 100 K, along the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line of the $\sqrt{3} \times \sqrt{3}$ SBZ in the $A_{||}$ geometry (see inset). (a) with 30° incidence angle; (b) with 30° incidence angle, but with a scan direction perpendicular to the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line near the $\bar{K}$ point ($\theta_e = 17.5^\circ$, see inset).

investigate the difference, we show spectra recorded along a direction perpendicular to the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line near the $\bar{K}$ point. Figure 4(b) shows a series of spectra obtained with a 30° incidence angle. The analyzer was set to a horizontal emission angle of 17.5° (θ_h), and the vertical angle (θ_v) was scanned. In similarity with Fig. 2(c), Fig. 4(b) also shows an obvious split between the two surface states for small deviations from the $\bar{K}$ point. We find a close resemblance between our 2.5° off spectrum and the $\theta_e = 18^\circ$ spectrum in Fig. 4 of Ref. 5.

To be able to trace any small change of S_2 and S_3 near the $\bar{K}$ point, we have investigated ARPES spectra with various incidence angles. Figure 5 shows two series of ARPES spectra obtained at RT and LT (100 K). We found that 25° is a suitable incidence angle since it results in a similar intensity for S_2 and S_3 . It is directly evident from the raw data that the RT spectra are essentially the same as the LT ones. These spectra once again show that there is no spectral evidence of a split between S_2 and S_3 either at RT or at LT. The report in Ref. 5 of the split surface bands at the $\bar{K}$ point was intended as a support of the IET model that has currently been subjected to intensive studies.^{5,9,10,12-14} It was concluded that the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface exhibits a disorder-order phase transition from RT to LT, meaning that S_2 and S_3 are already split at room temperature. Since we find that the spectra do not show any detectable split, we have to conclude that a discussion of an order-disorder transition cannot be based on the photoemission data.

It is clear that our photoemission results do not agree with the predicted, large band splitting of the IET structure in Ref.

FIG. 5. ARPES spectra recorded with a photon energy of 21.2 eV at 100 K, along the $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ line of the $\sqrt{3} \times \sqrt{3}$ SBZ in the $A_{\perp}$ geometry (see inset). All the spectra were obtained around the $\bar{K}$ point with an incidence angle of 25° . (a) at room temperature; (b) at 100 K.

3 and 15. Since STM images clearly favor the IET model at low temperature, the obvious conflict between the predicted band split of 0.15 eV at the $\bar{K}$ point and our photoemission result is disturbing. However, a very recent theoretical study has presented a solution to this dilemma. In the paper by Chen *et al.*,¹⁶ the surface band structure of the IET model was reinvestigated. The split between S_2 and S_3 was calculated to about 0.04 eV, which is significantly smaller than the 0.15 eV split reported earlier. The difference was attributed to different exchange-correlation forms used in the two theoretical studies.^{3,16} This new theoretical estimate of the split (0.04 eV) makes the IET model consistent with the measured band structure around the $\bar{K}$ point since it is smaller than the detection limit of the photoemission experiment. The experimental polarization dependence indicates an even and odd character of the S_2 and S_3 bands along $\bar{\Gamma}$ - $\bar{K}$ - $\bar{M}$ in agreement with the initial study. However, the symmetry properties, as derived from the emission intensities, are not strictly odd or even, which may indicate a broken symmetry as predicted by the IET model. The above results indicate that there is no real contradiction between the photoemission data and the IET model provided the theoretical energy split is small.

In conclusion, the surface electronic structure of the Ag/Si(111) $\sqrt{3} \times \sqrt{3}$ surface has been investigated by ARPES. We find that neither the $A_{||}$ nor the $A_{\perp}$ geometry provides any spectral evidence that S_2 and S_3 are split at the $\bar{K}$ point at reduced sample temperatures down to 100 K. At first the absence of a split between the surface bands seems to rule out the IET model. However, a recent theoretical re-

sult has turned this picture upside down. The very small calculated split of about 0.04 eV is consistent with the non-detectable split in our photoemission study, and there is no conflict with the IET model. As a consequence of the non-detectable split, one cannot base a discussion of a temperature-

dependent order-disorder transition on valence-band data around the $\bar{K}$ point.

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*Electronic address: hanmin.zhang@kau.se

†Present address: Dept. of Physics, Karlstad University, S-651 88 Karlstad, Sweden.

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