Surface-state band structure of the $Si(100)2 \times 1$ surface studied with polarization-dependent angle-resolved photoemission on single-domain surfaces

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The electronic structure of the Si(100)2 \times 1 surface has been studied with polarization-dependent angle-resolved photoemission. By using vicinal Si(100) samples, single-domain 2×1 surfaces were obtained, and the surface-band dispersions were measured unambiguously along the symmetry axes $\overline{\Gamma} \cdot \overline{J}'$ and $\overline{\Gamma} \cdot \overline{J}$ in the surface Brillouin zone (SBZ). The obtained dispersions are compared to dispersions from earlier studies of two-domain surfaces, as well as to theoretical band-structure calculations. In addition to the well-known surface state attributed to the dangling bonds, five more surface-related structures were observed on the single-domain surface. One of these is the controversial surface state previously observed on two-domain surfaces at \bar{J}' in the [010] direction at ~ 0.9 eV below the Fermi level (E_F) , which is not accounted for in any calculated surface band structure for the Si(100)2 \times 1 surface. Contrary to a previous report, it is also observed on the single-domain surface at several points in the SBZ. The second additional structure was found to disperse downwards along the $\overline{\Gamma}$ - \overline{J}' line, to a minimum energy of 3.4 eV below E_F at \overline{J}' . It is interpreted as a back-bond resonance. The third additional structure was seen as a faint peak at the Fermi level in normal emission. Finally, two other surface-related structures were found in the $\overline{\Gamma}$ - \overline{J} direction, one at ~ -1.3 eV at $\overline{\Gamma}$ in the second SBZ, splitting into two peaks for higher \mathbf{k}_{\parallel} values. By using a linearly polarized light source, the symmetry properties of the surface states and resonances were determined along the symmetry axes $\overline{\Gamma} \cdot \overline{J}'$ and $\overline{\Gamma} \cdot \overline{J}$ in the SBZ. The polarization dependence for several states indicates a mirror symmetry along these directions, with the dangling-bond state having even parity in both directions, in agreement with theoretical predictions for symmetric dimer models, and the back-bond resonance having odd parity in the $\overline{\Gamma} \cdot \overline{J'}$ direction. Three of the surface states and resonances are not accounted for in theoretical band structures for the 2×1 reconstruction. Two of these can be explained by domains of asymmetric dimers, arranged into $c(4 \times 2)$ or $p(2 \times 2)$ periodicities.

I. INTRODUCTION

The clean Si(100) surface normally exhibits a 2×1 low-energy electron diffraction (LEED) pattern, as first reported by Schlier and Farnsworth.¹ The basic element of this reconstruction is by now well established. It consists of dimers formed in the top atomic layer, i.e., two atoms in the top layer bond to each other, thereby reducing the number of dangling bonds on the surface by half, compared to the ideal, unreconstructed surface.

However, many questions regarding the details of the reconstruction are still not resolved, e.g., the minimumenergy atomic geometry, differences between the calculated and experimental surface band structures, the importance of defects, magnetic ordering, etc. One major question is whether the dimers are parallel to the surface (symmetric [see Fig. 1(a)] or buckled (asymmetric)). Surface band-structure calculations² based on the originally proposed symmetric dimer model gave two overlapping dangling-bond bands, resulting in a metallic surface, whereas the results of angle-resolved photoemission experiments³ showed that the surface is semiconducting. With buckled dimers, first introduced by Chadi,⁴ the two dangling-bond bands are split further apart, resulting in a surface band gap, in agreement with experiments. This



FIG. 1. (a) Drawing of a symmetric dimer model for the $Si(100)2 \times 1$ surface. (b) The surface Brillouin zones of the single-domain surface in the repeated zone scheme. Symmetry points are indicated in the figure. Mirror planes of the surface are indicated with dashed lines.

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model can also explain the reports of $c(4 \times 2)$ and (2×2) reconstruction elements on the surface from LEED (Refs. 5-8) and He diffraction⁹ studies, as well as the observed phase transition from 2×1 to $c(4 \times 2)$ when cooling the surface.¹⁰ By now, most theoretical total-energy calculations have favored atomic geometries with asymmetric di-mers,¹¹⁻¹⁶ with some significant exceptions.^{17,18} Pandey¹⁷ also found a substantial decrease in the surface total energy by introducing missing dimer defects on the surface. Very recently, Artacho and Ynduráin,¹⁸ based on cluster calculations and earlier Si 2p core-level photoemission studies,¹⁹ proposed that symmetric dimers have the lowest total energy due to an antiferromagnetic spin arrangement within the dimers. Experiments with structural techniques like low-energy²⁰ and mediumenergy²¹ ion scattering have supported the dimer model, but have not distinguished between symmetric and asymmetric dimers.

Important information about the Si(100)2×1 surface has in recent years been obtained with the scanningtunneling-microscopy (STM) technique.²² The STM studies showed that the surface reconstruction consists mainly of symmetric dimers, together with a high density of defects and asymmetric dimers around some of the defects.

The electronic structure of the $Si(100)2 \times 1$ surface has been studied extensively with angle-resolved photoelectron spectroscopy (ARPES) (see Ref. 23 for a recent review), as well as with inverse photoemission²⁴ and electron-energy-loss spectroscopy (EELS).^{25,26} So far, five different surface states or resonances have been identified in different ARPES studies. The most prominent of these is the dangling-bond state. Two other states have been associated with the dimer bond. $^{27-29}$ However, two of the surface states are not accounted for in the theoretical band structures calculated so far, for either symmetric or asymmetric 2×1 dimer models. One of these states has been observed in several ARPES studies around \bar{J}_{2}^{\prime} [\bar{J}^{\prime} in the second surface Brillouin zone (SBZ); see Fig. 1(b)] in the [010] direction, at ~ 0.9 eV below the Fermi level (E_F) . A second unexplained surface state has been seen at the Fermi level, in normal emission and near \overline{J}'_2 on highly *n*-doped samples,³⁰ and in normal emission on *p*doped samples.³¹

The previous ARPES studies of the $Si(100)2 \times 1$ surface have been complicated by the two-domain nature of the surface, caused by the existence of single atomic layer steps, which rotate the reconstruction by 90°. The superposition of contributions from the two types of domains on the surface makes band mapping of the surface states along the symmetry directions in the SBZ difficult and ambiguous. Therefore, in most ARPES studies, the surface-state dispersions have been measured along the diagonal [010] direction [see Fig. 1(b)], which is common to both domains. However, as described by Kaplan,³² it is possible to obtain a single-domain 2×1 -reconstructed surface by the use of vicinal Si(100) samples, with the offorientation tilting towards a $\langle 011 \rangle$ direction. After careful preparation of these samples, terraces separated by double atomic-layer steps are formed, thereby giving the single-domain surface. Single-domain $Si(100)2 \times 1$ surfaces have also been obtained on on-axis cut samples by growth of buffer layers with the molecular-beam epitaxy (MBE) technique and high-temperature annealing.³³

In the present experiment we have studied the singledomain $Si(100)2 \times 1$ surface with ARPES, using samples cut 4° off the (100) plane, tilting towards [011]. The formation of the single-domain surface has allowed us to determine the dispersions and symmetry properties of the surface states unambiguously in the main symmetry directions of the surface. A detailed comparison is made to the surface-state dispersions obtained on the twodomain surface, as well as to theoretical band-structure calculations. The five earlier reported surface states are identified also on the single-domain surface. In particular, contrary to the report of Bringans, Uhrberg, Olmstead, and Bachrach,³⁴ the controversial surface state ob-served at \bar{J}'_2 at ~ -0.9 eV on two-domain surfaces was identified also on the single-domain surface, at several points in the SBZ. By the use of linearly polarized light, the symmetry properties of the surface states and resonances have been examined. The observed polarization dependence for several of the surface states is in good agreement with the symmetry properties expected for symmetric dimer models.

II. EXPERIMENTAL DETAILS

The ARPES experiments were performed in a UHV chamber with a base pressure of less than 2×10^{-10} Torr. The light source was a resonance lamp, providing photon energies of 16.85 and 21.2 eV. By deflecting the light in an osmium-coated mirror, a strong linear polarization in the horizontal plane was obtained. The hemispherical analyzer could be rotated in both the horizontal and the vertical planes. The angular resolution was $\sim \pm 1^{\circ}$, and the energy resolution was ~ 150 and ~ 200 meV, for 21.2 and 16.85 eV photon energy, respectively. The Fermi level (E_F) position was determined by photoemission from the metallic (Ta) sample holder.

The samples were made from an n^+ -doped, mirrorpolished Si single-crystal wafer ($\rho = 4-6 \text{ m}\Omega \text{ cm}$, Asdoped, Wacker-Chemitronic), cut 4° off the (100) plane, tilting towards the [011] direction. Before insertion into the vacuum chamber, they were cleaned using the etching procedure of Ishizaka and Shiraki.³⁵ In ultrahigh vacuum they were thoroughly outgassed at 600-750 °C and then cleaned by stepwise heating up to 850 °C. After each annealing, the samples were cooled down in 2-3 minutes. After 2 min at 850 °C, a good single-domain 2×1 LEED pattern was obtained. The formation of regularly spaced double-layer steps was indicated by the characteristic splitting of the LEED spots, as described by Kaplan.³² To maintain the clean surface, the samples were annealed for 30 s at \sim 800 °C every second hour. No sign of contamination was seen in the ARPES spectra within this time period. Spectra are also presented from ARPES experiments on the two-domain Si(100)2×1 surface, using $(\rho = 4$ n^+ -doped $m\Omega cm$, As-doped, Wacker-Chemitronic) on-axis cut samples and the same sample preparation as described above.

Complementary ARPES experiments were done on the

single-domain hydrogen-chemisorbed Si(100)2×1:H surface³⁶ and on the two-domain (on-axis) Si(100)2×1 surface.²⁹ Additional ARPES experiments were also done with synchrotron radiation at Hamburger Synchrotron-strahlungslabor (HASYLAB), Deutsches Elektronen-Synchrotron (DESY), on both single- and two-domain Si(100)2×1 surfaces.³⁷

In order to explore the polarization dependence of the surface-state emission, ARPES spectra were recorded with three different geometries: With normal incidence of the light, the polarization vector was either *in* the plane defined by the [100] direction and the emission direction, or essentially *perpendicular* to the same plane. This will be referred to as the A_{\parallel} case and the A_{\perp} case, respectively. For spectra recorded with a high angle of incidence ($\theta_i = 60^\circ$), the component of the polarization vector parallel to the surface was directed according to the A_{\parallel} case. All the angles of incidence (θ_i) and emission (θ_e) given in this article refer to the [100] direction and *not* to the surface normal for the off-oriented samples.

III. EXPERIMENTAL RESULTS

ARPES spectra from the single-domain Si(100)2×1 surface are presented in Figs. 2, 3, 6, and 7. In Fig. 2, a collection of spectra, recorded in the [011] direction (i.e., the direction perpendicular to the dimer bonds) for different experimental conditions, is shown. The emission angle is chosen in order to show the electronic states near the \overline{J}' point in the SBZ [see Fig. 1(b)]. An angular series of spectra, recorded with the A_{\perp} geometry in the same azimuthal direction, is presented in Fig. 3. The structure denoted A in the spectra is the well-known surface state associated with the dangling bonds. It is ob-



FIG. 2. ARPES spectra, recorded with 16.85 eV photon energy in the [011] direction. The recording geometries are indicated in the figure. The emission angle $(\theta_e = 30^\circ)$ is chosen in order to show the electronic states near the \bar{J}' point in the SBZ. Spectrum (a) was recorded on the Si(100)2×1:H surface (Refs. 36 and 38). The labels of the peaks are explained in the text.



FIG. 3. ARPES spectra, recorded with 16.85 eV photon energy and the A_{\perp} geometry in the [011] direction (the $\overline{\Gamma}$ - \overline{J} ' line in the SBZ). The labels are explained in the text. For the lowest spectrum, the angle of incidence (θ_i) was 10° and for the other spectra, $\theta_i = 0^\circ$.

served with the strongest emission intensity for high angles of incidence, but can be clearly seen also with the A_{\parallel} geometry near \overline{J} ' [Fig. 2(c)]. In the corresponding A_{\perp} spectrum [Fig. 2(b)], the A peak is strongly suppressed and instead two other surface-related structures are observed, denoted B and D. The assignment of these peaks to surface states or resonances is supported by the comparison to the corresponding spectrum from the $Si(100)2 \times 1$:H surface [Fig. 2(a)], where peaks B and D are missing. [As described in Ref. 38, the 2×1 :H spectrum (a) was shifted in order to compensate for the different E_F position on this surface.] The structures C and E are identified as bulk transitions. Structure C is discussed in detail below. The dispersions of peaks B and D can be followed in more detail in the spectra in Fig. 3 and their initial energies as a function of the wave vector $[E_i(\mathbf{k}_{\parallel})]$ are plotted in Fig. 4. Also the dispersion of the dangling-bond state, recorded with the A_{\parallel} geometry, is shown in Fig. 4. The dangling bond (peak A) can also be seen in the A_{\perp} spectra in Fig. 3, as a faint peak for intermediate emission angles and contributing to the rather strong peak for the lowest emission angle. This is due partly to the nonperfect linear polarization of the light and partly to the nonzero angle of incidence that was used for the $\theta_e = 15^\circ$ spectrum, because of technical constraints.

In the $[01\overline{1}]$ direction $(\overline{\Gamma} \cdot \overline{J} \cdot \overline{\Gamma}_2)$, the direction parallel to the dimer bonds; see Fig. 1), the dispersion of the dangling-bond band is almost flat, with a bandwidth of ~0.1 eV, as seen in Fig. 5. The polarization dependence of the dangling bond at $\overline{\Gamma}_2$ is illustrated in Fig 6. The peak denoted A at ~0.8 eV below E_F is the danglingbond peak. Another peak, denoted H, is seen at ~ -1.3 eV at $\overline{\Gamma}_2$. Beyond that point, it splits into two peaks, one



FIG. 4. Dispersions of the surface states and resonances in the [011] direction on the single-domain Si(100)2×1 surface, recorded with 16.85 eV photon energy. The recording geometries are indicated in the figure. Also shown are the calculated surface bands, based on an asymmetric dimer model, from Ref. 13. The labeling of the theoretical bands is taken from a private communication from J. Pollmann. The shaded region is the projected bulk band structure (Ref. 13). For the Fermi-level position, the value $E_F - E_V = 0.6$ eV was used (Ref. 38).

almost nondispersive and one denoted I, that disperse steeply downwards, as illustrated in Figs. 5 and 7. Both these peaks are highly sensitive to hydrogen adsorption, as can be seen by comparing the two uppermost spectra in Fig. 7. A small part of the H peak emission at $\overline{\Gamma}_2$ is due to an overlap with a bulk peak. A strong direct bulk transition, seen in normal emission at this initial energy with 16.85 eV photon energy, is surface umklapp scattered to $\overline{\Gamma}_2$, as was shown in Ref. 36. The bulk contribu-



FIG. 5. Dispersions of the surface states and resonances in the $[01\overline{1}]$ direction on the single-domain Si(100)2×1 surface. The $\theta_i = 45^\circ$ data are recorded with the photon energies 13 and 15 eV, and the A_{\parallel} and A_{\perp} data with 16.85 eV. The dispersion of the A peak could be followed also in the A_{\parallel} spectra, but has been omitted in this figure for clarity. The dashed line is the projected bulk band edge for the 1×1 SBZ. For the other details in the figure, see the caption to Fig. 4.



FIG. 6. ARPES spectra, recorded with 16.85 eV photon energy in the [011] direction. The recording geometries are indicated in the figure. The emission angle $[\theta_e = 30^\circ;$ for spectrum (b), $\theta_e = 31^\circ$] is chosen in order to show the electronic states near the $\overline{\Gamma}_2$ point in the second SBZ. Spectrum (d) was recorded on the Si(100)2×1:H surface (Refs. 36 and 38). The labels of the peaks are explained in the text.

tion is shown in spectrum (d) in Fig. 6, recorded from the Si(100)2×1:H surface with the A_{\perp} geometry. The strength of the bulk emission was roughly the same in the corresponding A_{\parallel} spectrum.

Also in the $[01\overline{1}]$ direction, the dangling bond is strongly suppressed in the A_{\perp} spectrum, as well as the Hpeak, and instead a broad peak, denoted B', is seen at ~ -1.1 eV [spectrum (c) in Fig. 6]. Taking into account the surface umklapp scattered bulk contribution, the B'peak appears to be at roughly the same energy as the Bpeak in the [011] direction and is clearly separated from the A and H peaks. The dispersion of the B' peak is also plotted in Fig. 5. Finally, the C peak seen in the A_{\perp} spectra in Fig. 6, is the same bulk transition that is observed in the [011] direction (Figs. 2 and 3).

The electronic structure at the \overline{K} point in the SBZ has also been probed on the single-domain surface (data not shown here). The dangling-bond state was found at -1.3eV at \overline{K} . The high-energy side of this peak has a pronounced shoulder, indicating another peak at ~ -0.9 eV.

It is interesting to compare the electronic structure of the single-domain Si(100)2×1 surface with the more commonly studied electronic structure of the two-domain surface. In Fig. 8 ARPES spectra, recorded in the [010] direction on both single- and two-domain surfaces, are shown. The emission angle corresponds to \mathbf{k}_{\parallel} points near



FIG. 7. ARPES spectra, recorded with 16.85 eV photon energy and the A_{\parallel} geometry in the [011] direction (the $\overline{\Gamma}$ - \overline{J} line in the SBZ). The labels are explained in the text. The uppermost spectrum was recorded on the Si(100)2 \times 1:H surface (Refs. 36 and 38).



FIG. 8. ARPES spectra, recorded in the [010] direction with 21.2 eV photon energy, from (a) the single-domain surface and (b)-(d) the two-domain surface on on-axis cut, low n-doped (Ref. 38) (b) and n^+ -doped (c)-(d) samples. Spectrum (b) was recorded from the Si(100) 2×1 :H surface (Ref. 29). The emission angle $(\theta_{e}=35^{\circ})$ was chosen in order to show the states near the \overline{J}_{2}' point in the second SBZ. The labels are explained in the text.

 \overline{J}_{2} (in the second SBZ). The structures A, B'', D', and F are identified as surface states or resonances, and structure G will be discussed as a possible surface resonance. The remaining peak in spectrum (b), denoted E', is identified as a bulk transition. The dispersions of the surface-related states on the two-domain surface is presented in Fig. 9. [The projected bulk band structure in Fig. 9 was obtained from a band-structure calculation using the linearized augmented plane-wave (LAPW) method.³⁹] A is the dangling bond and B'' is the controversial state discussed earlier, that cannot be accounted for in band-structure calculations for 2×1 dimer models. As seen in spectrum (a) in Fig. 8, it is present also on the single-domain surface. Structure D' is a surface resonance, dispersing downwards towards \bar{J}'_2 . The D' structure is sensitive to hydrogen adsorption, as seen in spectrum (b), and it has also been identified in spectra recorded with 15 and 16.85 eV photon energy (not shown here), which further supports its identification as a surface resonance. In the normal-incidence spectrum (d), the D' peak is hardly visible, indicating that the D' emission is strongly dependent on the z component of the polarization vector of the light. Structure G, dispersing sharply around \bar{J}_{2} , has been suggested as a surface resonance since its dispersion is insensitive to photon energy and symmetric with respect to the SBZ, and it appears in the projected 1×1 bulk band gap.^{29,31} This structure was observed also on the Si(100)2×1:H surface, but not on the 3×1-H surface, which led to the suggestion that it is associated with the dimer bonds on both the 2×1 :H and the clean 2×1 surfaces.²⁹ The nature of this state is discussed further below.

Structure F is the surface state observed at the Fermi level at $\overline{\Gamma}$ and \overline{J}' on two-domain (n^+ -doped) surfaces.³⁰



FIG. 9. Dispersions of the possible surface states and resonances in the [010] direction on the two-domain $Si(100)2 \times 1$ surface. The difficulties in positively identifying structure G are discussed in the text. The data were recorded with 21.2 eV photon energy from an n^+ -doped sample. The recording geometries are indicated in the figure. The shaded region is the projected bulk band structure, from Ref. 39. The dashed line shows the projected bulk band edge for the 1×1 SBZ. The value $E_F - E_V = 0.6$ eV was used (Ref. 38) for the Fermi-level position.

This state was seen also on the single-domain $(n^+$ -doped) surface, but with very much lower intensity, and was therefore only observed in normal emission. With 21.2eV photon energy, a faint peak could be observed, but with 16.85 eV photon energy it could not be resolved. A possible explanation for the lower intensity on the single-domain surface is the expected higher density of defect states (e.g., step-related states), which could deplete the charge in the Fermi state. Due to the weak emission, no information about its polarization dependence could be obtained. In an earlier ARPES study on the two-domain surface, ³⁰ the F state was found to have p_z character.

As seen in Figs. 4 and 9, the dispersions of the dangling-bond state in the [011] and [010] directions on the single- and two-domain surfaces, respectively, are very similar. The initial-energy position at $\overline{\Gamma}$ is slightly higher on the single-domain surface, indicating a different Fermi-level position, which is consistent with the absence of the Fermi-level state on this surface. The bandwidth of the dangling-bond band is also slightly different: 0.7 eV on the single-domain surface and 0.75 eV on the two-domain surface.

Comparing the electronic states at \overline{J}_2' on the two-domain surface to the states at \overline{J}' on the single-domain surface, it is easy to identify the B state at \overline{J} i as the B'' state at \overline{J}_{2} . Similarly, the energy positions and dispersions of the D and D' peaks in Figs. 4 and 9 clearly show that they originate from the same band. However, the different polarization dependence for this resonance in the [011] and [010] directions is striking. In the [010] direction, the D' peak appears to have a strong p_z character, whereas in the [011] direction, the D peak is only observed with the A_{\perp} geometry. The polarization dependence of the B and B' peaks in the [011] and $[01\overline{1}]$ directions, respectively, is difficult to determine, due to the partial overlap with the dangling bond, but it does not appear to be strong. The fact that the B and B' peaks at \overline{J} ' and $\overline{\Gamma}_2$ are seen clearly only with the A_{\perp} geometry may be due to the strong emission from the dangling bond (peak A) with the other geometries. The initial energies and the flat dispersions for the B, B', and B'' peaks indicate that they all originate from the same surface state (in the following discussion denoted with B only). The pronounced shoulder seen at -0.9 eV at \overline{K} is most likely another contribution from the same state. For low emission angles, this B state overlaps with the dangling bond and cannot be identified.

A closer examination of the data in Fig. 9 shows that the *B* state actually has a finite dispersion. This can be seen more clearly in spectra recorded with higher resolution from a cooled two-domain surface of an n^+ -doped sample. Those spectra are presented in Fig. 10. The sample was cooled to ~160 K and spectra were recorded in the [010] direction with 21.2 eV photon energy. The total experimental resolution was ~75 mV. The main effect of the cooling was a sharpening of the surface-state peaks and a strong increase in the emission intensity of the Fermi-level state. The dominant reason for this is the sharpening of the Fermi-Dirac distribution function. The *B* state also appeared slightly stronger. It has previously been reported that a phase transition from 2×1 to



FIG. 10. High-resolution ARPES spectra recorded in the [010] direction with 21.2 eV photon energy from a two-domain, on-axis sample. The sample was n^+ -doped and cooled to ~160 K. The total resolution was estimated to be 75 meV.

 $c(4\times2)$ occurs when cooling the Si(100)2×1 surface.¹⁰ This was not observed in the present experiment, but in the LEED pattern, faint streaks were observed near the $\frac{1}{4}$ -order position on the cooled surface, indicating the onset of a phase transition.

Due to the sharpening of the surface-state peaks, a dispersion of at least 0.15 eV can be seen for the *B* peak in the spectra in Fig. 10. Also, in the normal emission spectrum, a broad structure at ~ -1.0 eV can be resolved from the dangling-bond peak. The existence of this structure has been suggested in earlier ARPES studies.^{3,37} Its energy position makes it probable that it is the same *B* state that is observed at $\overline{\Gamma}_2$ in the [011] direction. However, due to the broadness of this structure, there may also be other contributions to the emission, as discussed below. The spectra in Fig. 10 also show the narrow angular intervals around $\theta_e = 0^\circ$ and 34° (corresponding to $\overline{\Gamma}$ and \overline{J}'_2 , respectively), where the *F* peak is observed.

The proposed surface resonance G, observed around \overline{J}'_{2} in the [010] direction, is expected to be found also around \overline{J}' in the [011] direction on the single-domain surface. At that \mathbf{k}_{\parallel} point, the structure denoted C in Figs. 2 and 3 appears, at the same initial energy as G. However, this peak is also observed at $\overline{\Gamma}_{2}$ in the [011] direction (Fig. 6), as well as on the 2×1:H and 3×1-H surfaces, which indicates that it is a bulk transition. A detailed inspection of peak C's dispersion also shows that it does not seem to follow the symmetry of the 2×1 SBZ, and that it splits into two peaks for high \mathbf{k}_{\parallel} values, as observed in Fig. 3. This peak is strongest for the \mathbf{k}_{\parallel} values corresponding to \overline{J}' and $\overline{\Gamma}_{2}$, which in the bulk Brillouin zone both correspond to a line passing through the L symmetry point. We therefore attribute this peak to emission from the uppermost valence band, which is almost flat along this line.³⁹ The initial energy for peak C at \overline{J} ' then gives a value of ~1.5 eV below the valence-band maximum (E_V) for the L'_3 point in the bulk band structure, in good agreement with earlier results.⁴⁰ The nearly flat valenceband dispersion (0.13 eV) along this line also has the effect that the initial energy of this bulk peak at the \mathbf{k}_{\parallel} value corresponding to \overline{J}' will be quite independent of photon energy. Calculated bulk direct transitions from this valence band to free-electron final bands show that the same is true also for the dispersion around \overline{J} ', in the photon-energy range 14-21.2 eV, in good agreement with the experimental dispersions for structure C from twodomain surfaces.³⁷

The above-stated observations make the assignment of peak G to a surface resonance questionable. Although this peak appears in the 1×1 bulk band gap in the [010] direction, it may originate from the C bulk transition at \overline{J}' , being umklapp scattered with a surface reciprocal lattice vector to \overline{J}'_2 . The same insensitivity to the photon energy as for peak G also occurs for peak C, and the symmetric dispersion of G around \overline{J}'_2 can be explained by surface umklapp scattering of C from \mathbf{k}_{\parallel} points near both of the two opposite \overline{J} ' points in the first SBZ. This alternative interpretation of peak G is also consistent with the fact that G is observed at \overline{J}'_2 on the 2×1:H surface, but is missing at the same \mathbf{k}_{\parallel} point on the 3×1-H surface, since on the 3×1 -H surface, peak C cannot be surface umklapp scattered from \overline{J}' to the \mathbf{k}_{\parallel} point corresponding to \overline{J}_{2} on the 2×1:H surface, due to the different periodicity.

IV. DISCUSSION

A large number of ARPES studies of the $Si(100)2 \times 1$ surface have been done previously (see review in Ref. 23). However, very few previous studies on a single-domain surface have been done.^{16,34} In a very recent theoretical study¹⁶ experimental dispersions corresponding to structures A, B, and H, obtained on a single-domain surface, were included. In Ref. 34 the dispersion of the dangling bond was presented. Comparing the dispersions of the dangling-bond band in the $\overline{\Gamma}$ - \overline{J} and $\overline{\Gamma}$ - \overline{J} ' directions in the present study to the previous results, we find a very good agreement. The main difference is the bandwidth in the $\overline{\Gamma}$ - \overline{J} ' direction, which was found to be 0.8 eV in Ref. 16, 0.6 eV in Ref. 34, and 0.7 eV by us. These results are also in good agreement with the dangling-bond dispersions for two-domain surfaces in the literature, as summarized in Ref. 23, and add up to a very consistent picture of this surface-state band.

The *B* state has been observed in practically all ARPES studies in the [010] direction on the two-domain surface. In the previous ARPES study of the single-domain surface of Ref. 34, this state was not observed at \overline{J}' and it was suggested that the *B* peak observed at \overline{J}'_2 on twodomain surfaces could be due to some second-order effect. However, as shown above, the *B* peak can be resolved at \overline{J}' when the photoemission from the dangling bond is suppressed in the A_{\perp} geometry. In fact, this state appears to be present in large parts of the SBZ.

The surface resonance denoted D (and D') is most likely the same state as the peak in Ref. 27 denoted C', and the S_3 state in Ref. 28. However, in those experiments, this state was only observed around the $\frac{1}{2}\overline{J}\,\overline{K}$ point, in the [010] direction. The full dispersion of the D' peak could not be recorded due to technical constraints: too low photon energy²⁷ and too small incidence angle for high emission angles,²⁸ respectively. In the ARPES study of Goldmann *et al.*³¹ a peak assigned to a direct bulk transition was found at \overline{J}'_2 at about the same initial energy as the D peak. In that work the D peak emission at \overline{J}'_2 was suppressed for the same reason as in Ref. 28. We note that a bulk peak (denoted E') is found close to the D peak position also in the present work, as seen in spectrum (b) in Fig. 8.

In Figs. 4 and 5 the dispersions of the surface-related structures in the [011] and $[01\overline{1}]$ directions are compared to the surface bands from the recent band-structure calculation of Pollmann et al., 13 based on an asymmetric dimer model. The dispersion of the A peak agrees fairly well with the D_{up} band, associated with the dangling bond on the upper dimer atom, although the calculation overestimates the bandwidth of the dangling-bond band in the $\overline{\Gamma}$ - \overline{J} ' direction. The D-band dispersion agrees well with the dispersion of the B_2 back-bond surface resonance. In Refs. 27 and 28 it was suggested that the D state, observed only around $\frac{1}{2}\overline{J}\,\overline{K}$, was associated with the dimer bond. As seen in Fig. 4, our results compared to theory do not support that view for the full dispersion of the D band. It can be noted, however, that the theoretical B_2 band and dimer band (D_i) overlap halfway between $\overline{\Gamma}$ and \overline{J} '.

As stated earlier and as seen in Figs. 4 and 5, the B state cannot be accounted for in the theoretical band structure for the 2×1 reconstruction. The energy position of the H peak around $\overline{\Gamma}_2$ in the [011] direction coincides with the calculated position of the B_1 back-bond resonance, as seen in Fig. 5. However, there is some uncertainty regarding the interpretation of this peak: the Hpeak may also be a contribution from the other domain, which may exist on a minor fraction of the surface, in which case the H peak would be the dangling bond, probed at \overline{J}' . We find this interpretation unlikely, since there was no indication of a contribution from the other domain in the [011] direction, at \overline{J} ', and since the LEED images were essentially single domain. If instead the Hpeak is associated with the B_1 resonance, one would expect to see this state also in normal emission, at $\overline{\Gamma}$ in the first SBZ. As shown above, a broad structure is actually seen near the H-peak energy in the normal emission spectrum from the cooled sample (Fig. 10). Although its peak position agrees better with the energy of the B state, a contribution at the *H*-peak energy, -1.3 eV, is possible, due to the broadness of the structure. This state seems to be present also in the dispersion presented in Ref. 16 and it was suggested that it may be a dangling-bond state from domains of asymmetric dimers on the surface, arranged into $c(4 \times 2)$ or $p(2 \times 2)$ periodicities.

The steeply dispersing I peak, which is split off from

the *H* peak beyond $\overline{\Gamma}_2$, cannot be associated with any corresponding calculated surface-resonance band,¹³ as seen in Fig. 5. However, this structure was found to be strongly sensitive to hydrogen adsorption, as illustrated in Fig. 7, and it has also been observed with other photon energies (14, 16, and 19 eV) on two-domain surfaces, with overlapping dispersions. We conclude that the assignment of the *I* peak to another surface resonance is the most likely interpretation.

Comparing our experimental results to the older theoretical band-structure calculation of Ihm, Cohen, and Chadi,¹¹ a better agreement than in Ref. 13 is found regarding the bandwidth of the lower (filled) danglingbond band, but the absolute-energy position is too high. Also in that calculation, a surface resonance was found dispersing downwards along $\overline{\Gamma}$ - \overline{J} ', in fair agreement with the D band in Fig. 4. In both Refs. 11 and 13 the dispersions for the dangling-bond bands in symmetric dimer models were also calculated. Comparisons to experimental results clearly favor the asymmetric dimer models in those calculations. However, other earlier calculations^{2,4} have given dangling-bond bands for symmetric dimers in good agreement with experiment, regarding the shape of the dispersions and bandwidths. When comparing the absolute energies and the energy separation between the upper and lower dangling-bond bands to experiment, the asymmetric dimer models are invariably favored. But this is not a very strong argument for asymmetric rather than symmetric dimers, considering the well-known inability to calculate correctly the fundamental band gaps in semiconductors and insulators with the widely used local-density approximation for correlation and exchange. Also, in a recent theoretical work¹⁸ it was asserted that the spin interaction within the dimers results in a gap between the dangling-bond bands for symmetric dimers and makes this model energetically favorable.

The earlier-discussed structure denoted G, dispersing around \overline{J}'_2 in the diagonal [010] direction on the twodomain surface, has previously been associated with the dimer bond.²⁹ While the energy position at \overline{J}'_2 is about 0.6 eV higher than the position of the theoretical dimer band D_i , at \overline{J}' (see Fig. 4), there is a qualitative agreement between G and D_i in that both disperse to a maximum at \overline{J}'_2 and \overline{J}' , respectively. However, as discussed above there are good reasons for questioning the surfaceresonance nature of structure G. Presently, our data are not sufficient to determine conclusively the nature of structure G.

The symmetry properties of the symmetric dimer model for the Si(100)2×1 reconstruction were discussed in detail in the early theoretical study of Appelbaum, Baraff, and Hamann.² The reconstruction has a mirror plane symmetry in the [011] and [011] directions, as indicated in Fig. 1. The electronic states with \mathbf{k}_{\parallel} vectors in a mirror plane are either even or odd under reflection in that mirror plane. It was found in Ref. 2 that the two dangling-bond orbitals on the dimer bind to each other in a π bond, forming antibonding and bonding combinations (π_a and π_b). The states in the antibonding (π_a) band thus have odd symmetry in the mirror plane containing the [011] direction, which bisects the dimer bond [see Fig. 1(a)], and even symmetry in the mirror plane containing the $[01\overline{1}]$ direction, whereas the states in the lower-energy, bonding (π_b) dangling-bond band have even symmetry in both mirror planes.

STM studies²² have shown that the Si(100)2×1 reconstruction consists predominantly of symmetric dimers. It was noted, however, that the STM images may show time-averaged flipping asymmetric dimers. In later STM studies⁴¹ the surface electronic states were studied in more detail. It was found that images reflecting the filled states and empty states on the surface, respectively, are quite different and indicate different symmetries for the filled and empty states, with the empty states having a nodal plane between the dimer atoms. These states were identified as the bonding (π_b) and antibonding (π_a) combinations of the dangling bonds, associated with the symmetric dimer model, in good agreement with the theoretical study of Appelbaum *et al.*²

The polarization dependence of the surface states that is observed in the present study can be explained by the existence of mirror-plane symmetries in the [011] and $[01\overline{1}]$ directions. According to mirror-plane selection rules,⁴² photoemission within a mirror plane from even initial states is suppressed with the A_{\perp} geometry and, conversely, emission from odd states is suppressed with the A_{\parallel} geometry. These rules, applied to the results presented in Figs. 2 and 6, indicate that the A state (dangling-bond) has even symmetry in both the [011] and $[01\overline{1}]$ directions, in agreement with the STM results and the theoretical predictions for the low-energy, filled dangling-bond band in a symmetric dimer model. Similarly, the H peak seen in the $[01\overline{1}]$ direction appears to have even symmetry with respect to the mirror plane containing the $[01\overline{1}]$ direction.

The polarization dependence of the *D* resonance indicates an odd symmetry for this band in the mirror plane containing the [011] direction. In the [010] direction, where the mirror-plane selection rules do not apply, the *D'* peak appears to have a strong p_z character. The interpretation of this band as a back-bond surface resonance is consistent with the calculation of Appelbaum *et al.*² in which a back-bond state with odd symmetry was found at $\overline{J'}$ at -2.86 eV.

No surface band-structure calculation, based on models of an ideal, dimerized 2×1 -reconstructed surface, has given a surface band that can be associated with the Bstate. This fact suggests that the B state is associated with imperfections on the surface, e.g., steps, point defects, or local higher-order reconstructions. STM studies of the Si(100)2×1 surface have invariably shown a high density of defects on the surface.^{22,43,44} Even on the best-prepared surfaces, the point-defect density is ~5%. 43,44 Another deviation from the ideal 2×1 reconstruction, observed in STM images, is small domains of asymmetric dimers around some of the point defects. Caution must be exercised when comparing the defect densities observed in STM images with possibly defectrelated states in ARPES spectra, since the sample preparation procedures in the various experiments were different. At the same time we emphasize that the intensity of, e.g., the B state seems very insensitive to the details of the surface preparation, as judged by the consistency in the results reported by different groups.

The fact that a finite dispersion is observed in the [010] direction for the B peak indicates that this state is quite delocalized. This conclusion excludes the point defects as the origin of the B state. Steps on the surface can be regarded as a type of extended defect. Due to the regularly spaced double-layer steps on the single domain, 4° off oriented surface, the amount of dangling bonds on the steps can be estimated to be $\sim 10\%$ of the dangling bonds on the terraces. The density of step-related states on an on-axis, two-domain surface is more difficult to estimate, but judging from STM studies, it may be considerably smaller. Also several different types of steps coexist on the two-domain surface, e.g., two types of single-layer steps. The similar, relatively strong intensities of the Bpeak on the single- and two-domain surfaces, therefore, seem inconsistent with an assignment to step-related states. A possible interpretation of the B peak is that it is associated with the dangling bonds in small domains with asymmetric dimers, as suggested in the very recent theoretical study of Zhu, Shima, and Tsukada.¹⁶ Asymmetric dimers are observed in STM images in regions of the surface with a relatively high number of defects and are arranged into local $c(4 \times 2)$ or $p(2 \times 2)$ periodicities in small areas with a typical size of at least 30 Å. It is possible that, with the sample preparation used in the present study, even larger areas with asymmetric dimers exist. In Ref. 16 it was shown that the dispersion of the B state is consistent with the calculated dispersions for the dangling bonds in a model with asymmetric dimers, arranged into either $p(2 \times 2)$ or $c(4 \times 2)$ periodicities.

Similar to the *B* state, the Fermi-level state, seen on the n^+ -doped two-domain surface, is difficult to reconcile with band-structure calculations for the 2×1 reconstruction. The peak at E_F near \overline{J}'_2 can be explained as the minimum of the upper, almost empty dangling-bond band, but not the peak at $\overline{\Gamma}$. For example, in the calculated band structure in Ref. 13, the energy position of the upper dangling-bond band at $\overline{\Gamma}$ is 0.55 eV higher than at $\overline{J'}$.

It has been suggested that this peak originates from point-defect states on the surface,³¹ in accordance with the interpretation of a similar surface state on the $Ge(100)2 \times 1$ surface.⁴⁵ These defect states would be associated with the disordered arrangement of asymmetric dimers. Another defect interpretation has been suggested in a recent STM study,⁴³ where one type of point defect was found to have localized electronic states at the Fermi level. However, due to the sharp localization of the Fpeak in \mathbf{k}_{\parallel} space around $\overline{\Gamma}$, it was argued in Ref. 30 that this peak should be attributed to the minimum of an intrinsic, dispersive surface-state band. The sharp angular localization of this state can be seen in Fig. 10. For normal emission, the full width at half maximum (FWHM) value in $k_{\|}$ space for the F-peak emission intensity is smaller than 0.14 Å $^{-1}.$ It was suggested in Ref. 43 that the sharp orientational dependence of the emission could be a consequence of the symmetry of the point defects. We find this explanation unlikely, considering the highly narrow angular interval for the emission (FWHM of 4°).

We are not aware of any example, in experiment or theory, of a spatially strongly localized state with a comparable angular dependence of the photoemission. It is interesting to note that around these point defects, regions of asymmetric dimers were observed in the STM images. It is possible that delocalized, bandlike states are pinned by the defects, leading to the localized appearance reported in the STM study.⁴³ In the calculated band structures for the energy-optimized $c(4 \times 2)$ and nonoptimized $p(2\times 2)$ reconstructions,¹⁶ the lowest empty dangling-bond band has a minimum at $\overline{\Gamma}$. It is thus possible that the F peak at $\overline{\Gamma}$ originates from band states, associated with the domains of asymmetric dimers, similar to the interpretation of the B state. This is also consistent with the intensity increase for this peak upon cooling. The F peak at \overline{J} ' could, on the other hand, originate from the dominating 2×1 reconstruction.

In view of the present knowledge about the $Si(100)2 \times 1$ surface, an interpretation of the B state and F state at $\overline{\Gamma}$ as originating from extended "defects" like the asymmetric dimer regions appears to be the most plausible explanation. However, it is clear that further studies are needed to determine conclusively the nature of these states. Of particular interest are studies of the electronic states associated with the defects observed in the STM studies, e.g., combined ARPES and STM studies of the same surface. Studies of the $c(4 \times 2)$ -reconstructed surface, obtained upon cooling, should also give very valuable information about the reconstruction and should be a critical test for the intepretation of the B and F states. Surface band-structure calculations using many-body theory may also be valuable. However, it is unlikely that a many-body calculation for the 2×1 -reconstructed surface will give a band structure where it will be possible to assign the B state or the F state at $\overline{\Gamma}$ to intrinsic surface bands.

The presented ARPES data indicate that the experimental surface contains a mixture of 2×1 domains with symmetric dimers and domains with higher-order reconstructed asymmetric dimers $[c(4\times 2) \text{ or } p(2\times 2)]$, in agreement with the STM studies.²² The polarization dependence of most of the surface states indicates the existence of symmetry properties that favor the symmetric dimer model for the main part of the surface, as discussed above. For an asymmetric 2×1 dimer model, there would be no mirror-plane symmetry in the [011] direction. The comparison between theoretical and experimental surface band structures favor to some extent the asymmetric 2×1 dimer model, but that is not a strong argument for this model, considering the similarity of calculated dangling-bond dispersions for symmetric and asymmetric dimers and the difficulty in calculating accurate values for surface-state band gaps. On the other hand, the existence and dispersions of the B and F peaks imply that there are domains of asymmetric dimers on a mirror part of the surface, arranged into higher-order reconstructions, as observed in STM studies²² and in agreement with recent theoretical work.¹⁶

V. SUMMARY

The $Si(100)2 \times 1$ surface has been studied with polarization-dependent angle-resolved photoemission. By

using vicinal Si(100) samples, single-domain 2×1 surfaces were obtained. The dispersions of the surface states and resonances were measured along the symmetry axes Γ -J ' and $\overline{\Gamma}$ - \overline{J} in the SBZ and were compared to the dispersions obtained in the diagonal $\overline{\Gamma}$ - \overline{J}'_2 direction on two-domain surfaces, as well as to theoretical band-structure calculations based on dimer models. The dispersion of the most prominent surface state, the dangling-bond state, was found to be in good agreement with both theory and earlier ARPES studies. In the [011] direction, a surface resonance was found, dispersing down to -3.4 eV at \bar{J}' , and interpreted as a back-bond resonance. In the $[01\overline{1}]$ direction, another surface resonance was found at -1.3eV at $\overline{\Gamma}_2$ (in the second SBZ), possibly also associated with the back bonds. Beyond $\overline{\Gamma}_2$, another surface-related structure is split off from this state and disperses steeply downwards. The interpretation of a previously reported surface resonance, observed dispersing up to -2.0 eV at \bar{J}_{2} in the diagonal [010] direction on two-domain surfaces, was questioned. An alternative interpretation was suggested, implying that this peak is a surface umklappscattered bulk transition.

Overall, a fair agreement between experiment and theory was found. One important exception is a surface state seen in large parts of the SBZ at ~ -0.9 eV. Another significant exception is a surface state seen at the Fermi level, highly localized in \mathbf{k}_{\parallel} space around $\overline{\Gamma}$ and \overline{J}'_{2} , when using n^+ -doped, on-axis cut samples. The peak

at E_F near \overline{J}'_2 can be explained as the minimum of the upper, almost empty dangling-bond band, but not the peak at $\overline{\Gamma}$. These two exceptions, however, can be explained by the existence of domains with asymmetric dimers on the surface, arranged into $c(4\times 2)$ or $p(2\times 2)$ periodicities.

The polarization dependence of the surface states and resonances associated with the 2×1 reconstruction indicates a mirror-plane symmetry in the [011] and [011] directions ($\overline{\Gamma} \cdot \overline{J}$ ' and $\overline{\Gamma} \cdot \overline{J}$ in the SBZ), with the dangling-bond state having even parity in both directions, in good agreement with theoretical predictions for symmetric dimer models.

Note added in proof. The ARPES results from singledomain $Si(100)2 \times 1$ surfaces included in Ref. 16 were very recently presented in an article by Enta *et al.* [Y. Enta, S. Suzuki, S. Kono, and T. Sakamoto, J. Phys. Soc. Jpn. **59**, 657 (1990)].

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the present work, $E_F - E_F = 0.4$ eV. Spectra (a) in Fig. 2, (d) in Fig. 6, and the uppermost spectrum in Fig. 7 are therefore shifted by 0.3 eV to lower binding energy to facilitate comparisons to the other spectra. For the same reason, spectrum (b) in Fig. 8 is shifted by 0.2 eV to higher binding energy.

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FIG. 4. Dispersions of the surface states and resonances in the [011] direction on the single-domain Si(100)2×1 surface, recorded with 16.85 eV photon energy. The recording geometries are indicated in the figure. Also shown are the calculated surface bands, based on an asymmetric dimer model, from Ref. 13. The labeling of the theoretical bands is taken from a private communication from J. Pollmann. The shaded region is the projected bulk band structure (Ref. 13). For the Fermi-level position, the value $E_F - E_V = 0.6$ eV was used (Ref. 38).



FIG. 5. Dispersions of the surface states and resonances in the $[01\overline{1}]$ direction on the single-domain Si(100)2×1 surface. The $\theta_i = 45^\circ$ data are recorded with the photon energies 13 and 15 eV, and the A_{\parallel} and A_{\perp} data with 16.85 eV. The dispersion of the *A* peak could be followed also in the A_{\parallel} spectra, but has been omitted in this figure for clarity. The dashed line is the projected bulk band edge for the 1×1 SBZ. For the other details in the figure, see the caption to Fig. 4.



FIG. 9. Dispersions of the possible surface states and resonances in the [010] direction on the two-domain Si(100)2×1 surface. The difficulties in positively identifying structure G are discussed in the text. The data were recorded with 21.2 eV photon energy from an n^+ -doped sample. The recording geometries are indicated in the figure. The shaded region is the projected bulk band structure, from Ref. 39. The dashed line shows the projected bulk band edge for the 1×1 SBZ. The value $E_F - E_V = 0.6$ eV was used (Ref. 38) for the Fermi-level position.