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Similarity of Si(110)5×1 and Si(111)2×1 surfaces

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Angle-resolved photoelectron spectroscopy has been used to study the electronic structure of Si(110) surfaces. On the 5×1 reconstructed surface a dangling-bond band with a dispersion of 0.35 eV is found. In a comparison with the dangling-bond band on Si(111)2×1 there are several similarities, which are discussed in terms of the common chainlike structures of the ideal Si(110) surface and the π-bonded chain model of Si(111)2×1.

Studies of the geometrical and electronic structure of silicon low index surfaces have attracted a lot of interest recently.[1–6] Both experimental and theoretical studies have mainly considered the (111) and (100) faces, while the (110) face has been largely neglected.

There are at least two reasons why the electronic and structural properties of the Si(110) surface deserve a closer examination. First of all, the (110) surface is the cleavage face of the III-V compounds, like GaAs and GaP, whose surface properties are fairly well understood.[7,8] In this context it is interesting to compare surfaces having the same ideal structure but differences in covalency and ionicity. The second reason is that the uppermost planes in Pandey's model[2] of the Si(111)2×1 surface have a chainlike structure which resembles the atomic configuration of the ideal (110) surface. One is then led to speculate that the surface electronic properties of these two surfaces could be similar, at least insofar as the reconstructed (110) surface maintains a chainlike structure.

In order to test this hypothesis, we have carried out angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) measurements on Si(110) surfaces with different reconstructions. In Fig. 1 we show the geometry of the unreconstructed (110) surface. The surface layer contains chains of silicon atoms having two bonds along the chain and one bond towards the second-layer chain. One electron per surface atom might form a π-bonding chain similar to what occurs in the π-bonded chain model of the Si(111)2×1 surface. The differences in geometry for these two surfaces are primarily the distance between the chains that is 5.43 Å on the (110) surface and 6.65 Å on Si(111)2×1, and the height separation between first- and second-layer chains that is much larger on the (110) surface than on Si(111)2×1.

The surface Brillouin zone of the unreconstructed (110) surface is shown in Fig. 1(b). We have studied the electronic structure along the long axis $\bar{\Gamma}\bar{X}$ and the short axis $\bar{\Gamma}\bar{X}'$. It is established that the dangling-bond band along the corresponding long axis ($\bar{\Gamma}\bar{J}$) on Si(111)2×1 has a strong positive dispersion of ≈ 0.7 eV in the outer half of the surface Brillouin zone.[4,5] As will be shown below, the Si(110)5×1 reconstructed surface has a similar dangling-bond band with a positive dispersion of 0.35 eV.

Previous experimental work on the clean Si(110) surface has mostly been concerned with structural analysis by low-energy electron diffraction (LEED).[9,10] Angle-integrated photoelectron spectroscopy studies have also been done on chemisorption of hydrogen on the Si(110)5×1 surface.[11]

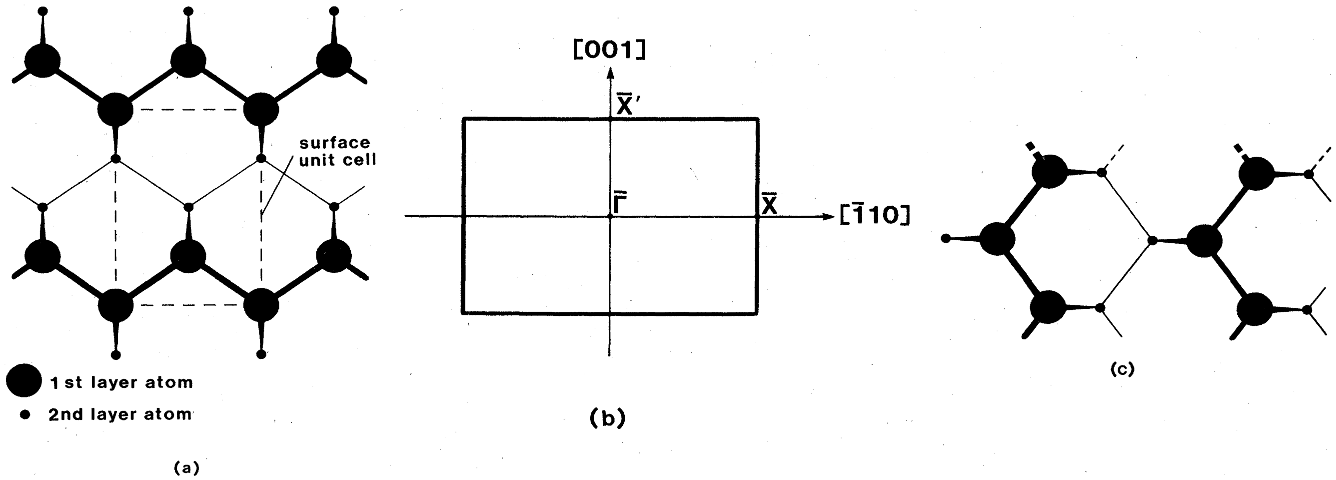

FIG. 1. (a) Geometry of the ideal Si(110) surface. (b) Geometry of the Si(110) surface Brillouin zone. (c) Side view of the ideal Si(110) surface. Dangling bonds are drawn as dashed lines.

The Si(110) surface exhibits several reconstructions, mainly depending on heat treatment, cooling rate, and history. As in the earlier studies[9-11] we have found it difficult to reproducibly obtain good LEED patterns following any of the recipes quoted in the literature. We have obtained reasonably good patterns for the 5×1 structure in the following way. The crystals were cleaned in ultrahigh vacuum (base pressure 1×10^{-10} torr) by repeated cycles of argon ion sputtering and thermal treatments ($\approx 1150\,^{\circ}\mathrm{C}$). By annealing for several minutes at 900 °C and then cooling rapidly we often obtained a good LEED pattern for the 5×1 reconstruction, while annealing at 700 °C resulted in facetting of the surface as evidenced by a complicated *X* LEED pattern.[9,10,12] The 5×1 surface has a fivefold increase of the surface unit cell perpendicular to the chains implying that the surface chains are not all identical, but some of them may be similar to the unreconstructed chains.

The present angle-resolved photoemission studies have been done using radiation from a hydrogen discharge lamp connected to a 225 McPherson monochromator. The details of the spectrometer have been published elsewhere.[6] ARUPS data for the main azimuthal directions $\bar{\Gamma}\bar{X}$ and $\bar{\Gamma}\bar{X}'$ [see Fig. 1(b)] have been collected for the clean and hydrogen exposed 5×1 and *X* structures using 10.2-, 9.0-, and 7.7-eV photon energies. Figure 2 shows the energy distribution curves (EDC's) of the emission from the Si(110)5×1 surface measured along the $\bar{\Gamma}\bar{X}$ direction for 10.2-eV photon energy.

In the corresponding set of spectra for the facetted *X* surface[13] it is possible to recognize the same main features appearing at higher binding energies than −1.5 eV in Fig. 2. Above −1.5-eV binding energy there are significant differences in the spectra which can be attributed to differences in the surface electronic structure of the two Si(110) surfaces. For the Si(110)5×1 surface we tentatively assign the structure *S* (Fig. 2) to be emission from a dangling-bond band which has similar characteristics as the dangling-bond band on Si(111)2×1.

By varying the angle of incidence of the photon beam (θ_i) the intensity of the dangling-bond emission changed, as can be seen in Fig. 3, curves a and c. The dangling-bond peak is minimum for $\theta_i=0$ indicating a p_z character of the wave functions, since it is excited by the A_Z component of the electric field. The interpretation of the peak as a surface feature is also supported by the sensitivity to hydrogen contamination. This can be seen in Fig. 3, where two EDC's at $\theta_i=65°$ and $\theta_e=40°$ are shown, one for the clean 5×1 surface (a) and one for the same surface after exposure to about 2×10^4 L (1 L $=10^{-6}$ torr sec) of hydrogen (b).[14]

For emission from the short axis $\bar{\Gamma}\bar{X}'$ we again find similarities with Si(111)2×1 since the surface state intensity is quite low in this direction for both surfaces and there is no clear dispersion of the surface state along the short axis on either surface.

In Fig. 4 we show the dispersion of the surface state *S* along $\bar{\Gamma}\bar{X}$. There is a total positive dispersion of 0.35 eV and the shape is consistent with a mirror symmetry around the Brillouin-zone boundary at $\bar{X}$. Figure 4 also shows the projection of the bulk bands of a self-consistent field linearized-augmented plane-wave (LAPW) calculation,[15] a value of $E_F-E_V=0.4$ eV has been used. It is clear that the surface state *S* is within the band gap in a large portion of the surface Brillouin zone. The similarities with the dangling-bond dispersion on Si(111)2×1 is striking, although the surface state feature on Si(110)5×1 is broader and the bandwidth is smaller. Since the quality of these two surfaces is quite different, i.e., the LEED patterns generally have sharper spots and less background on the Si(111)2×1 surface, the difference in peak width may partly be due to disorder effects.

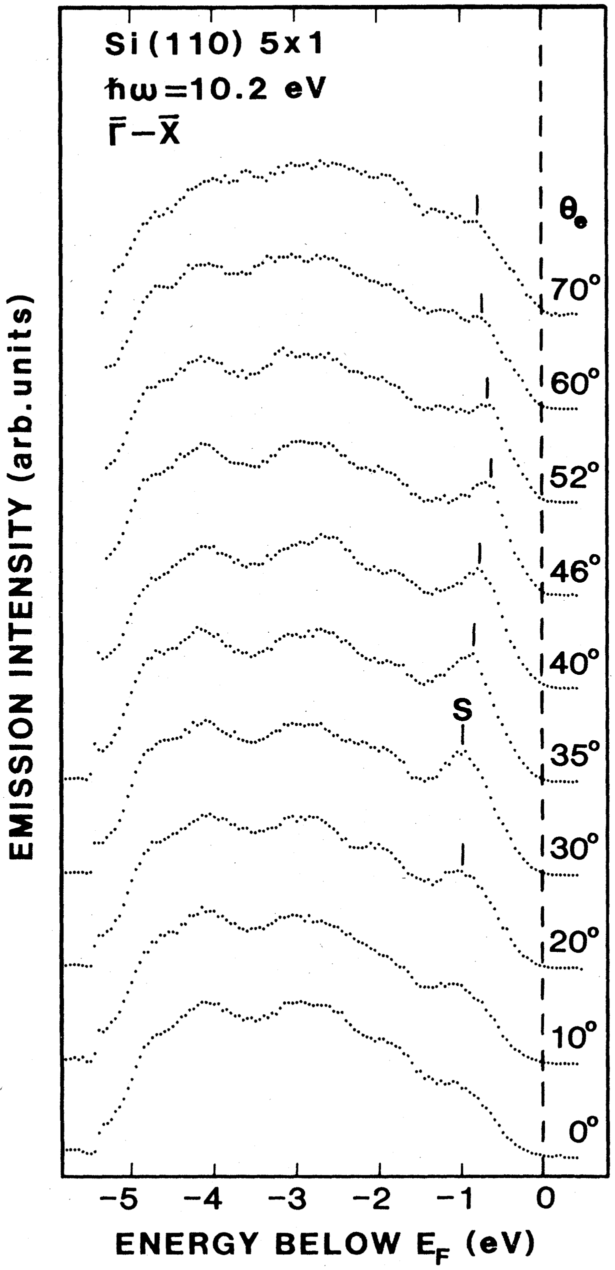

FIG. 2. Photoemission spectra for electrons emitted with $k_{\parallel}$ along the [110] direction. $\theta_i=65°$, except for $\theta_e=70°$ for which $\theta_i=45°$.

To try to understand the origin of the smaller bandwidth on Si(110) it is necessary to compare the geometries of Si(110) and Si(111)2×1 surfaces in more detail. On the ideal Si(110) surface the chain atoms are part of a sixfold ring [Fig. 1(c)], while on Si(111)2×1 they are part of a

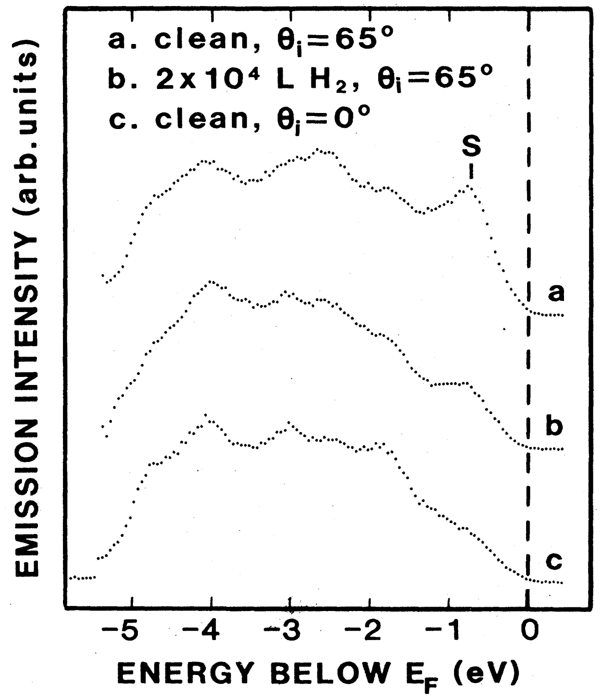

FIG. 3. Photoemission spectra supporting the dangling-bond interpretation of peak *S*. $\theta_e=40°$.

sevenfold ring (see, e.g., Fig. 1 in Ref. 3). This leads to a more planar geometry for the chain atoms and their back bonds on Si(111)2×1. The dangling bonds will thus be pointing out close to the normal direction. On the (110) surface the dangling bonds are much more tilted away from each other; the overlap is smaller resulting in a smaller bandwidth.

The Si–Si bond length is longer on the ideal (110) surface than on Si(111)2×1 (Ref. 3) also supporting a decrease in the bandwidth. However, only a detailed calculation of the atomic and electronic structure of the relaxed (and reconstructed) Si(110) surface can tell if the arguments above are valid.

A comparison of our results for Si(110)5×1 with the electronic structure of GaAs(110) shows clear qualitative differences. The dangling-bond band on this surface has a *negative* dispersion of ≈ 0.6 eV and remains within the projected bulk bands all along $\bar{\Gamma}\bar{X}$.[16] For GaAs(110) the reconstruction has ionic character; it involves dehybridization and charge transfer from Ga to As, so that dangling bonds sit mostly on second neighbor atoms. We suggest that the different dispersion of the dangling-bond band on Si(110)5×1 as compared with GaAs(110) is due to the formation of π bonds between the nearest-neighbor dangling bonds on Si(110)5×1.

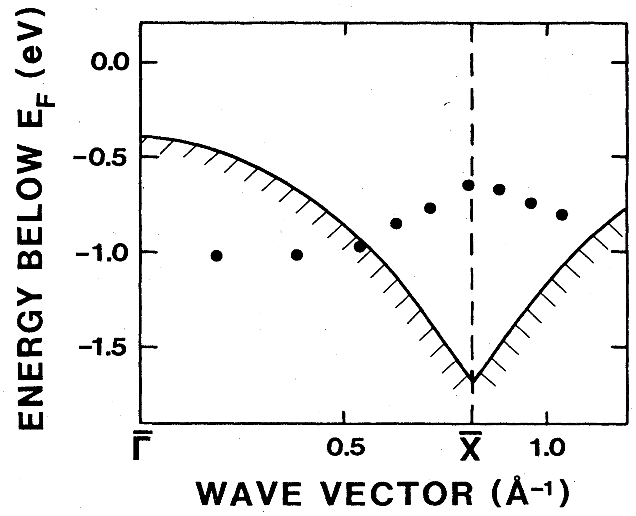

FIG. 4. Experimental dispersion of peak *S* relative to the edge of the projected bulk bands.

In conclusion, we have performed ARUPS studies on Si(110) surfaces exhibiting both 5×1 and *X* reconstructions. We have identified a dangling-bond band on the Si(110)5×1 surface which disperses upwards by 0.35 eV along the $\bar{\Gamma}\bar{X}$ direction. A comparison with spectroscopic data for the Si(111)2×1 surface points out a striking similarity between the electronic structures of these two surfaces. Since the atomic structure of the ideal Si(110) surface contains zigzag chains similar to the chains in Pandey's model for the Si(111)2×1 surface our results support the hypothesis that π-bonded chains are an essential part of the reconstructed Si(110)5×1 surface.

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