Detection of a Fermi level crossing in three-domain Si(111)-In(4×1)

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Using photoemission and inverse photoemission, it has recently been demonstrated that single domain Si(111)-In(4×1) overlayers possess a clear Fermi level crossing at $\approx 0.6\overline{\Gamma X}$. However, a previous inverse photoemission study, that was performed on a three domain sample, concluded that the overlayer was semiconducting. In an attempt to reconcile the results of the two inverse photoemission studies we proposed, in an earlier paper, that the first study did not probe the region of reciprocal space where the Fermi level crossing is now known to occur. In this paper we demonstrate that this suggestion is correct. Using a three domain Si(111)-In(4×1) overlayer, we mapped along the $\overline{\Gamma K}$ azimuth of the 1×1 zone, which is coincident with the $\overline{\Gamma X}$ azimuth of the 4×1 zone, with inverse photoemission, and found a Fermi level crossing at $\approx 0.6\overline{\Gamma X}$. We have now detected Fermi level crossings in both single and three domain 4×1 overlayers.
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INTRODUCTION

Of the seven In overlayer phases that have been observed on the Si(111) surface, in the coverage range that extends from 0.2–1.2 ML,[1–9] the 4×1 phase is arguably the most interesting. The In atoms order in rows that are either two or three atoms wide.[4,6,8–10] The electronic structure of the In rows has recently been shown to reflect the quasi-one-dimensional (quasi-1D) atomic structure.[11–13] The dispersion of the In-derived features in the valence and conduction bands is largest in the direction that is parallel to the In atom rows. The dispersion perpendicular to the atom rows is flat,[11–14] indicating that there is negligible wave-function overlap between the In atom rows. Consequently, the 4×1 system belongs to a small but fascinating class of quasi-1D overlayer systems. These systems are described as quasi-1D because they actually have a repeated chain structure, which resembles an atomic scale diffraction grating. The In rows are weakly interacting, so the system can be considered to be an array of isolated 1D atom wires. In fact, it is the repeated chain structure that actually allows us to study the electronic structure of the In atom rows with conventional spectroscopies that are not spatially resolved.

In studies of the 4×1 phase two issues have received a great deal of attention. The first issue, the registry of the In atoms on the Si(111) surface,[8,10,15] is still a subject of active study. The proposed surface structures divide into two classes. Those that place the In atoms on a largely unreconstructed Si(111) surface[8,15] and those that require the uppermost Si layer to reconstruct.[10] The second issue that has received attention is the nature of the electronic system. One of the first studies of the 4×1 phase, using inverse photoemission,[7] found it to be semiconducting. Inverse photoemission spectra collected from a three-domain sample at the zone center,[7,16] and also along the $\overline{\Gamma M}$ high-symmetry direction of the 1×1 surface Brillouin zone,[16] did not furnish evidence for a Fermi-level crossing. However, more recent studies performed on single-domain samples with photoemission[11] and with scanning tunneling microscopy (STM)[10,17] concluded that the overlayer was metallic. (Of course, this system may contain an energy gap below the experimental detection threshold. The system is quasi-1D and consequently it may exhibit a Peierl's instability. Furthermore, because of the low dimensionality of the system, it may not be a conventional Fermi liquid with a concomitant step in the momentum distribution function.) We also recently studied the single domain 4×1 phase with inverse photoemission[12–14] and found clear evidence for a Fermi-level crossing at $\approx 0.6\overline{\Gamma X}$. As far as the electronic structure of the overlayer is concerned, it is important to reconcile the results of the two inverse photoemission studies, which were performed on three[7,16] and single-domain 4×1 phases,[12–14] respectively. In an attempt to reconcile the two studies we proposed, in an earlier paper,[12] that the first study of the 4×1 phase did not discover a Fermi-level crossing because it did not probe the region of reciprocal space where the Fermi-level crossing is now known to occur. To test our hypothesis, we grew a three domain 4×1 overlayer phase on a Si(111) surface and mapped along the $\overline{\Gamma K}$ direction of the 1×1 zone, for reasons that we will now explain.

The C_{3v} symmetry of the Si(111) surface supports three 4×1 phases which can be mapped into one another by simple 120° rotations about the surface normal. The C_{3v} symmetry can be broken by using a vicinal Si(111) surface that contains steps. The relationship between the first Brillouin zones of the three 4×1 phases (labeled 1–3) and the Brillouin zone of the unreconstructed bulk 1×1 is illustrated in Fig. 1. First, consider the case where only one 4×1 domain exists (e.g., number 1). Then the $\overline{\Gamma K}$ symmetry direction of the 1×1 zone is coincident with the $\overline{\Gamma X}$ direction of the 4×1 phase. Furthermore, the orthogonal $\overline{\Gamma M}$ direction of the 1×1 zone (Fig. 1) is coincident with the $\overline{\Gamma X'}$ direction of the 4×1 phase. If there are three 4×1 domains present, the situation is more complicated. Mapping along the $\overline{\Gamma K}$ direction of the 1×1 zone now also samples low-symmetry directions of the other two 4×1 domains (2 and 3). The same is true for the $\overline{\Gamma M}$ direction. From Fig. 1, and

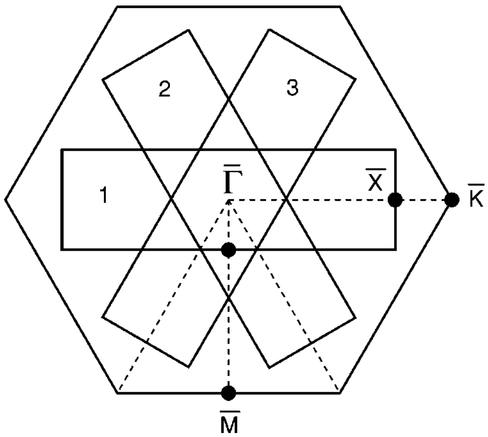

FIG. 1. The first Brillouin zone of the Si(111) 1×1 net is shown (outer hexagon) together with the first Brillouin zone of the 4×1 rectangular net in the three possible orientations. The three 4×1 zones are numbered 1–3 and referred to in the text. The $\overline{X'}$ symmetry label has not been included in the figure, because of space restrictions on the figure. Its location is indicated by a full circle.

the results of earlier studies[12–14] where we detected a Fermi-level crossing at $\approx 0.6\overline{\Gamma X}$, we predict that a Fermi-level crossing should appear along any of the $1\times1\,\overline{\Gamma K}$ directions if a three-domain overlayer is used. However, the intensity of the Fermi-level emission should be attenuated, by $\approx 1/3$, if

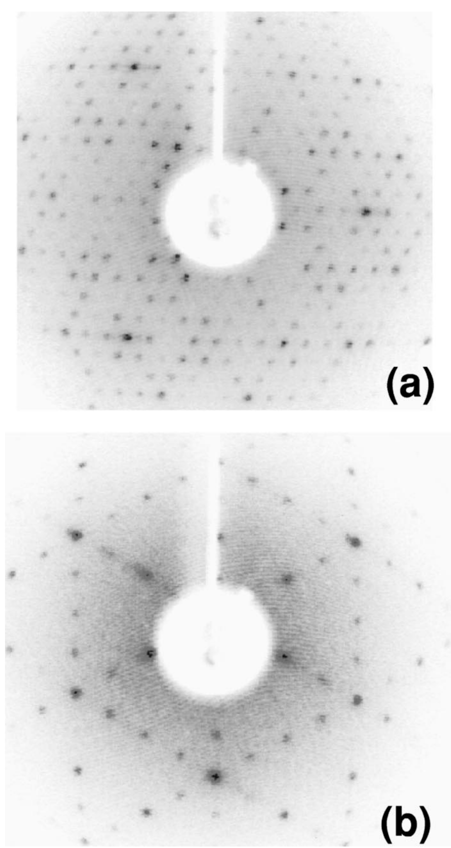

FIG. 2. Electron diffraction images collected from (a) the Si(111)7×7 surface immediately prior to In deposition and (b) the three domain Si(111)-In(4×1) phase. The kinetic energy of the electrons was 79.5 and 82.2 eV, respectively.

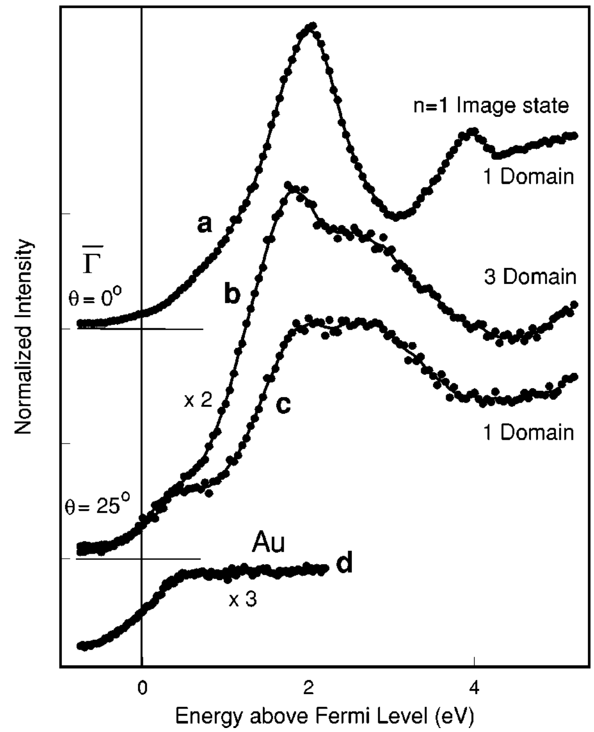

FIG. 3. Inverse photoemission spectra collected from (a) a single-domain 4×1 overlayer probed at the $\bar{\Gamma}$ point of the Brillouin zone, (b) for comparison with (c), a three-domain 4×1 overlayer probed with the electron gun 25° off-normal along the $\overline{\Gamma K}$ direction of the 1×1 zone, which is parallel with the $\overline{\Gamma X}$ direction of one of the 4×1 domains, (c) a single-domain 4×1 overlayer probed with the electron gun 25° off-normal along the $\overline{\Gamma X}$ direction, (d) the Fermi edge of a polycrystalline Au film. Curve (b) has been multiplied by 2 and curve (d) has been multiplied by 3. The superior signal-to-noise level of curve (a) is simply a consequence of a larger collection time.

all three phases are present in the same proportion and there is no contribution from higher lying states.

EXPERIMENT

The inverse photoemission experiments were performed with a low-energy electron gun[19] and a high sensitivity, Geiger-Müller bandpass photon detector,[18] which have been described previously.[12–14,18]

The single domain 4×1 overlayers were grown on vicinal *n*-type Si(111) wafers, with resistivities of $\approx 5\ \Omega$ cm, miscut by $3\pm0.5°$ towards $[\bar{1}\bar{1}2]$. Well-ordered 7×7 surfaces were created by resistively heating the substrates to $\approx 1050°$. The 4×1 overlayers were grown by depositing In onto the Si(111) surfaces heated to $\approx 395\,°C$. To align the Si(111) planes parallel with the front of the sample holder, the sample was mounted in a holder that counter-rotated it by the vicinal offcut angle. Although the three-domain overlayers can easily be grown on flat, nonvicinal Si(111) surfaces, we actually used the vicinal wafers described above to grow three-domain 4×1 overlayers. Occasionally the procedure that we outlined above would not produce a single 4×1 domain. Presumably, this is due to the fact that distribution of steps on the Si(111) surface is critically dependent upon the details of the flashing-annealing cycle. [Optimal annealing strategies for vicinal Si(111) surfaces are currently being developed.[20]] The three-domain 4×1 data that we present in this paper were all collected from vicinal Si(111) surfaces that had clear three-domain 4×1 electron diffraction patterns. We also attempted to produce 4×1 overlayers by depositing In on room temperature Si(111) and then post annealing. However, this produced a surface with both $\sqrt{3}\times\sqrt{3}R30°$ and 4×1 phases.[12]

RESULTS

An electron diffraction image collected at a kinetic energy of 79.5 eV from a clean Si(111)(7×7) surface is presented in Fig. 2(a). The image that is presented in Fig. 2(b) was collected at 82.2 eV from a three-domain 4×1 overlayer that was grown on the same surface. This can be compared with the single-domain 4×1 diffraction pattern that we previously published.[12]

In Fig. 3, we present inverse photoemission spectra that were collected from both the single domain 4×1 overlayer (a) and (c) and the three-domain 4×1 overlayer (b). Curve (a) probes the $\bar{\Gamma}$ point of the surface Brillouin zone whereas curves (b) and (c) were collected with the electron gun rotated 25° from the surface normal. In this geometry, the Fermi level is probed at $\approx 0.6\overline{\Gamma X}$. The emission at the Fermi level arises from a band (or a number of bands[11]) dispersing down towards the $\bar{X}$ Brillouin zone boundary where there is a binding energy maximum.[11] Curve (b) has been multiplied by a factor of 2 to line up the emission intensity in the Fermi-level region with the corresponding spectrum collected from the single-domain sample (c). Once again, there is emission at the Fermi level, indicating that there is a band crossing. However, the Fermi edge is harder to resolve because there is a broad intense feature located 1.8 eV above the Fermi level. In the absence of this feature, we would expect the Fermi-level emission intensity to be reduced by a factor of 3 in the three-domain 4×1 sample. The electron diffraction images from the three-domain surface [Fig. 2(b)] display approximately equal spot intensities from all three domains. Moreover, spectra collected from the three-domain system (not shown) along the $\overline{\Gamma X}$ line in the vicinity of $0.6\overline{\Gamma X}$ are qualitatively similar to single-domain spectra we have published previously.[12]

DISCUSSION

In a previous study of a single-domain 4×1 overlayer with inverse photoemission,[12,13] we found a clear Fermi-level crossing in the vicinity of the $\bar{X}$ zone boundary. Using the knowledge gained from this study, we have demonstrated, that it is also possible to detect the Fermi-level crossing using a three-domain sample. However, it is much more difficult to do so because only $\approx 1/3$ of the scattering volume contributes to the emission in the vicinity of the Fermi level. The previous inverse photoemission studies[7,16] of the 4×1 phase examined the $\bar{\Gamma}$ point and the $\overline{\Gamma M}$ direction of the 1×1 zone, which is orthogonal to the $\overline{\Gamma X}$ direction of the 4×1 zone (domain 1). This direction also samples two low-symmetry directions of the other two 4×1 domains (2 and 3). We have collected inverse photoemission spectra along the $\overline{\Gamma X'}$ direction of a single-domain 4×1 overlayer previously[13] and found that there are no bands that disperse across the Fermi level. Since the $\overline{\Gamma X'}$ direction is parallel to the $\overline{\Gamma M}$ direction of the 1×1 zone, we would not expect to see a Fermi-level crossing along $\overline{\Gamma M}$. Consequently, we believe that we have been able to reconcile the differences between the results of our inverse photoemission studies,[12,13] which were performed using single-domain overlayers, and the results of inverse photoemission studies performed on three-domain overlayers.[7,16] The results of both studies support the view that the electronic structure is quasi-1D and metallic.

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