Scanning tunneling microscopy of cleaved semiconductor surfaces

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Scanning tunneling microscopy is used to study the surface topography of cleaved GaAs(110) and Si(111) surfaces. For GaAs we observe 1 × 1 periodicity, with an [001] corrugation amplitude of typically 0.2 Å and a [$\bar{1}$10] corrugation amplitude of ~0.05 Å. Surface point defects are observed, consisting typically of ~0.7-Å-deep depressions extending along the rows. For Si(111), we find a periodicity of two unit cells, indicating the presence of the 2 × 1 reconstruction. We observe a maximum [2$\bar{1}\bar{1}$] corrugation amplitude of 0.5 Å and a [0$\bar{1}$1] corrugation amplitude of <0.02 Å, consistent with the π-bonded chain model for this surface. Structural disorder on the surface most commonly appears as "protrusions" along or crossing over between the chains. Orientational disorder is observed in the tilt of the chains.

1. Introduction

Owing to their great practical importance in device fabrication, semiconductor materials, and in particular the surfaces thereof, have been extensively studied by a wide variety of experimental techniques. The newest of these techniques is scanning tunneling microscopy (STM), which is unique in its ability to determine both structural and local electronic properties of these surfaces. The structural information is useful in determining the atomic positions on the surface, whereas the electrical information can lead to a microscopic view of Fermi-level pinning on the surface. The first semiconductor surface studied in detail by STM was the 7 × 7 Si(111) surface [1], and subsequent investigations have dealt with Ge(111) [2] and Si(100) [3] surfaces. In all of these studies the surfaces were prepared by *annealing* in vacuum. In this work, we present results on GaAs(110) and 2 × 1 Si(111) surfaces prepared by *cleaving* in vacuum. In the remainder of this section, we summarize the current view of the structure of these surfaces. This is followed by a description of our experimental apparatus and presentation of our results. In the final section, we compare our results for these two surfaces, illustrating the similarities and differences between them.

In its unrelaxed form, the GaAs(110) surface consists of "chains" of alternating Ga and As atoms directed in the [$\bar{1}$10] direction, as shown in **Figure 1(a)**. Each Ga and As atom binds a single electron in a half-filled dangling bond. When relaxed, the surface maintains its 1 × 1 periodicity, but the electrons in the Ga dangling bonds transfer to the As, thereby forming fivefold-coordinated As atoms and threefold-coordinated Ga atoms. Consequently, the As

atoms move out of the surface by about 0.65 Å relative to the Ga atoms [4–6]. This picture of the surface morphology, as first determined by low-energy electron diffraction (LEED), is consistent with our STM results [7]. In addition, we observe point defects in the form of ~0.7-Å-deep depressions along an atomic row.

The 2 × 1 reconstruction of the Si(111) crystal face has been the subject of numerous experimental and theoretical studies. It was originally thought that the reconstruction involved buckling of the surface atoms [8]. On the basis of a critical evaluation of experimental data and total energy considerations, Pandey proposed a radically new "π-bonded chain model" for the Si(111) surface [9]. In this model, the (111) surface reconstructs to form zigzag chains of atoms directed in the [01$\bar{1}$] direction, as shown in **Figure 1(b)**. A number of experiments support this particular model for the surface structure [10]. We have used STM to measure a maximum [2$\bar{1}\bar{1}$] corrugation amplitude of 0.5 Å together with no observable [01$\bar{1}$] corrugation. As discussed in [11], these values are consistent with the π-bonded chain model. Defect-related states have been previously observed on the 2 × 1 Si(111) surface, although the atomic structure of the defects was not known [12]. Here, we identify the dominant types of structural disorder on the surface to be atomic protrusions along the chains and protruding crossovers between the chains. We also observe disorder in the form of rigid tilts and/or translations of the chains.

2. Experiment

The tunneling microscope used in this work is similar to the "second-generation" microscope described by Binnig and Rohrer [13]. A two-stage spring suspension with magnetic damping supports a 10-cm-diameter base plate on which the microscope is mounted. Coarse motion is accomplished using a "louse" with $SrTiO_3$ insulators. Fine motion is accomplished with an *xyz* piezoelectric tripod with arm lengths of about 2.5 cm, resulting in a 1.3-kHz resonance frequency for the structure. Drift due to thermal expansion and/or piezoelectric creep is typically 3 Å/min, with about 5 min needed to acquire a 70 × 70-Å^2 image consisting of 100 × 100 data points. Hysteresis between opposite-direction scans is $\lesssim$1% of the scan length, and our images include data from both directions of a raster scan. In the GaAs image presented here, a running average has been performed on data from successive pairs of line scans. For all the other images no averaging has been employed. A least-squares-fit planar background including a quadratic term in the *y* direction has been subtracted from each image.

For our GaAs work, ground tungsten probe tips were used with no special tip-cleaning procedures. Our Si results were obtained using etched tungsten probe tips which were cleaned by passing large (μA) electron currents from tip to sample. All samples were cleaved *in situ* at a pressure of $<4 \times 10^{-11}$ torr. GaAs samples were cleaved in the [100] direction exposing a (110) crystal face, and Si samples were cleaved in the [2$\bar{1}\bar{1}$] direction exposing a (111) crystal face.

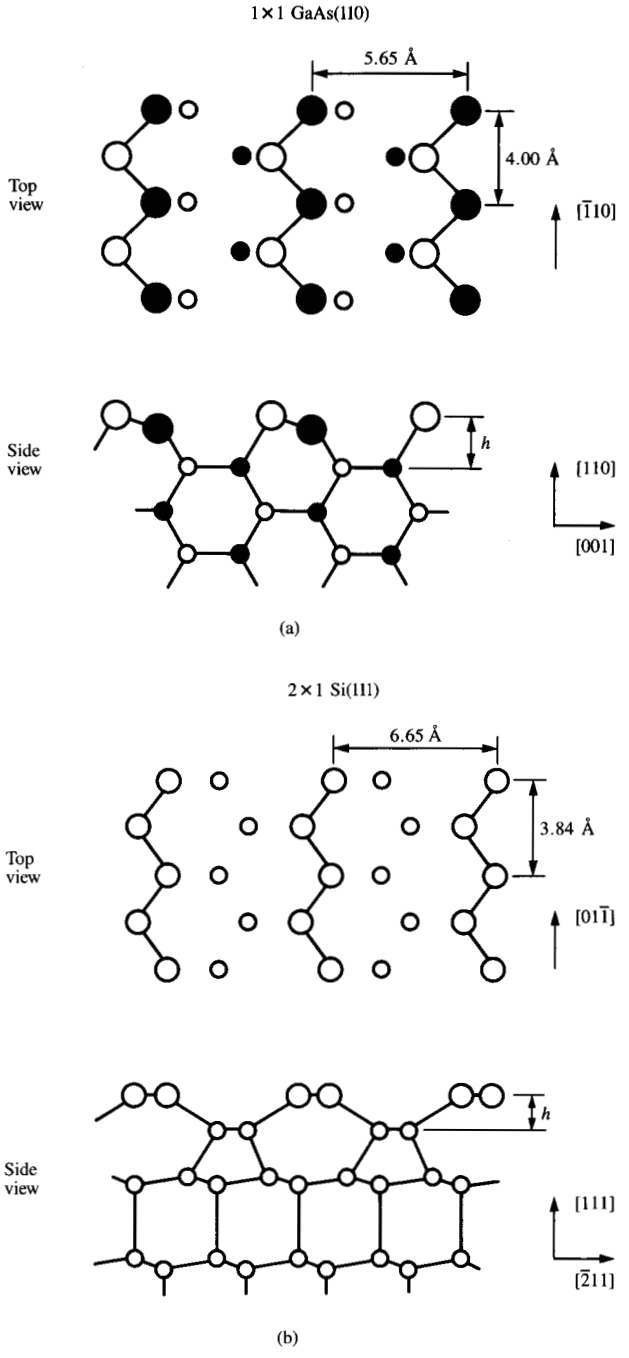

Figure 1

(a) Schematic view of the GaAs(110) surface. As atoms are shown in white, and Ga atoms are black. The separation *h* of the top two atomic layers is 2.1 Å [5]. (b) Schematic view of the π-bonded chain model for the 2 × 1 Si(111) surface. The separation *h* of the top two atomic layers is about 1 Å [10]. Figure 1(b) reprinted with permission from the *Journal of Vacuum Science and Technology*.

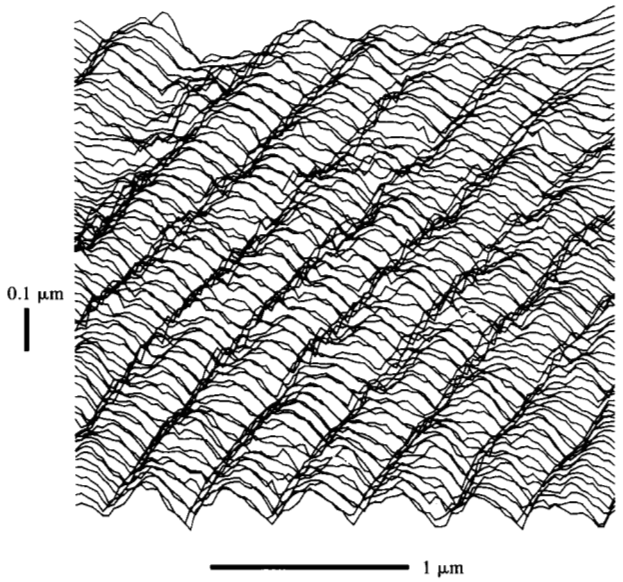

Figure 2

STM image of a gold-coated optical grating with a groove spacing of 2995 Å. The image extends laterally over an area of 2.8 × 2.8 μm^2, with the vertical height given by the scale on the left side of the figure.

GaAs material was p-type (Zn doped at 3×10^{18} cm^{-3}), and Si material was n-type (As doped at 2×10^{19} cm^{-3}). Evaporated Au contacts were used on the GaAs samples, and In contacts were used on the Si samples. In all cases the resistance of the contacts was negligible compared to the tunneling junction resistance. All measurements were performed with a constant tunneling current of 1 nA, and various bias voltages which are specified below.

Our first calibration of the tunneling microscope was performed using a gold-coated optical grating, with groove spacing of 2995 Å. **Figure 2** shows an STM image of the grating. By scanning independently with the x and y piezoelectric arms we were able to determine their calibration and also the absolute orientation of the grating. Then, by rotating the grating by 90° and scanning with the z arm using an L-shaped tip, we also calibrated that arm. Subsequent calibrations have been performed for the lateral direction by observing the lattice spacing of known materials, and for the vertical direction by using inductive "proximitors."

3. Results

• *GaAs(110)*

In **Figure 3(a)** we show an STM image of the GaAs(110) surface, acquired at a sample voltage of −3 V relative to the probe tip. Atomic rows running along the [$\bar{1}$10] direction are clearly visible. The vertical topography of these rows forms a major surface corrugation, with wavevector in the [001] direction, and a smaller corrugation with wavevector in the [$\bar{1}$10] direction. The peak-to-valley amplitudes of these corrugations, measured from the image, are 0.2 Å and ~0.05 Å, respectively. A numerical Fourier transform of the image is shown in **Figure 3(b)**. The major corrugation gives rise to the peak labeled (10), and the smaller corrugation gives rise to the (01) peak. The crystal was mounted with the [$\bar{1}$10] direction at 45° to the scan direction, and apparent deviations from this geometry in the image are due to drift effects. From the period of the corrugations measured along a given line scan, we deduce surface unit cell dimensions of

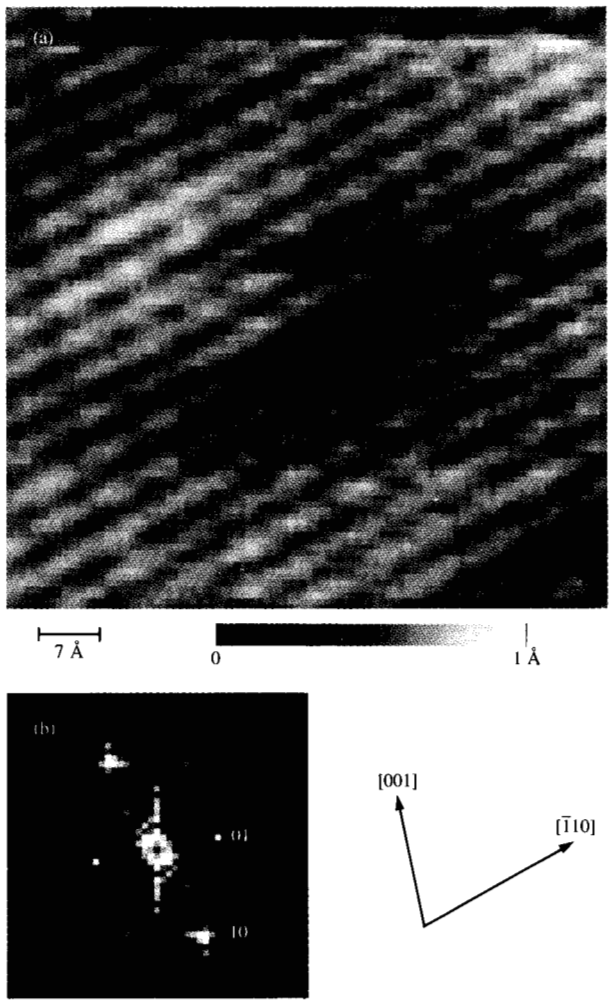

Figure 3

(a) STM image of a cleaved GaAs(110) surface. The image extends laterally over an area of 70 × 70 $Å^2$, with surface height given by the gray scale ranging from 0 (black) to 1 Å (white). An [001] corrugation with amplitude 0.2 Å is seen in the image, along with a [$\bar{1}$10] corrugation with amplitude ~0.05 Å. The lower (dark) region near the center of the image is a point defect. (b) A Fourier transform of the image. From [7], reprinted with permission.

6.5 Å × 5.0 Å, which are fairly close to the accepted values of 5.65 Å × 4.00 Å for 1 × 1 periodicity. We attribute the difference between these values to drift effects and a small calibration error.

The dark (lowered) area near the center of Figure 3(a) is due to a surface defect (another defect is seen in the lower right corner of the image). Similar defects have been seen in other images [7]. The defects typically consist of an ~0.7-Å-deep depression in the atomic row, with lateral dimensions of one unit cell in the [001] direction by about two unit cells in the $[\bar{1}10]$ direction. Since the atomic rows are aligned both vertically and laterally on all sides of the depression, the defect is *not* a dislocation, but rather, it is a point defect. We estimate the surface density of these point defects to be roughly 2×10^{12} cm^{-2}, which corresponds to a bulk density of 1×10^{20} cm^{-3}. Thus far we have only observed the defects on p-type samples which were Zn-doped (substitutional for Ga) to a density of about 3×10^{18} cm^{-3}. We do not know whether the observed defects are related to the Zn-doping.

• *Si(111)*

In **Figure 4** we present an STM image of the Si(111) surface, acquired with a sample voltage of +0.6 V relative to the probe tip. On the left side of the image are the atomic chains of the 2 × 1 reconstruction. The lateral spacing between the rows is measured to be about 6.9 Å compared to an actual value of 6.65 Å for a periodicity of two unit cells. The peak-to-valley corrugation amplitude for this $[2\bar{1}\bar{1}]$ corrugation is measured to be 0.5 Å. The image of Figure 4 actually displays exceptionally high resolution, while most other images at a bias of +0.6 V have a $[2\bar{1}\bar{1}]$ corrugation amplitude of typically 0.15 Å. We observe no $[0\bar{1}1]$ corrugation above our detection limit of 0.02 Å.

In addition to the 2 × 1 periodic structure observed by STM, we see disorder on the surface. Two classes of disorder are observed: First, we see structural disorder which typically has the form of protrusions ~1 Å high along or crossing over between chains. This is shown on the right-hand side of Figure 4, and also in the large-area scan of **Figure 5**. These protrusions are probably not due to sample contamination, since they have been repeatedly observed within 30 min (the time required to initiate the STM imaging) after cleaving the sample in a vacuum of $<4 \times 10^{-11}$ torr, during which time <0.04 monolayers of foreign atoms strike the Si surface. The surface density of structural protrusions seen in Figure 5 is about 7×10^{12} cm^{-2}, compared to a surface density of dopant As atoms (assuming a uniform distribution) of 3×10^{11} cm^{-2}. We have observed the structural protrusions on samples varying over a wide range of doping (9×10^{14} to 2×10^{19} cm^{-3} with As, P, and B dopants), and the protrusions density does not appear to be correlated with the doping level. Another type of disorder on the surface is seen in the asymmetry and magnitude of the $[2\bar{1}\bar{1}]$ corrugation. In Figure 4, for example, the atomic rows near the center of the image are clearly asymmetric, and this asymmetry varies across the image. We believe that this asymmetry indicates a *tilt* of the atomic chains. The tilts are observed to vary across the surface possibly in response to strain associated with nearby structural defects.

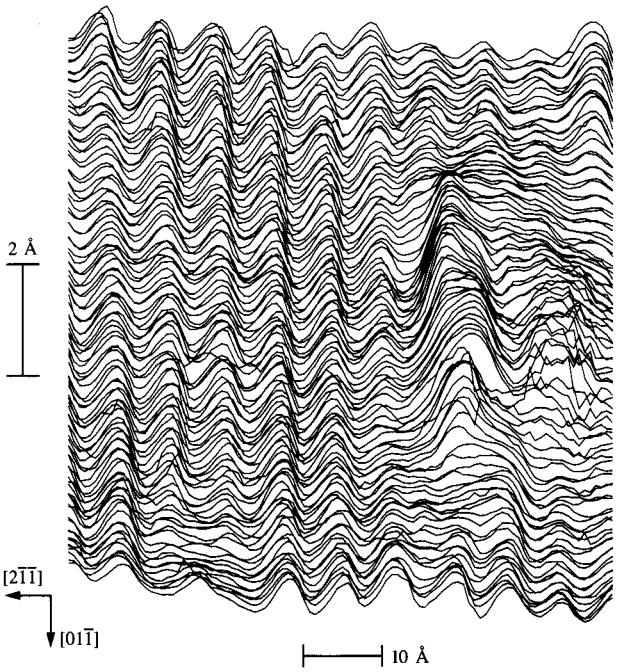

Figure 4

STM image of a cleaved Si(111) surface. The image extends laterally over an area of 70 × 70 Å^2, with the vertical height given by the scale on the left side of the figure. The 2 × 1 π-bonded chains are seen on the left side of the image, and a disordered region is seen on the right. From [11], reprinted with permission.

4. Discussion

In this section we compare our STM results for GaAs and Si. First we consider the amplitude of the corrugation observed for the two systems. The GaAs image presented in Figure 3 has a [001] corrugation amplitude of 0.2 Å; other images of that surface have corrugation amplitudes in the range 0.2–0.5 Å. The Si image of Figure 4 displays a $[2\bar{1}\bar{1}]$ corrugation amplitude of 0.5 Å; a more typical amplitude for that surface is about 0.15 Å. Thus, the corrugation amplitudes for the two surfaces are quite similar, which is not surprising since the atomic structures of the surfaces are alike. As shown in Figure 1, both surfaces consist of zigzag chains of atoms. The 2 × 1 reconstruction of the Si surface effectively converts the first two layers of that surface into a (110) structure.

Although the structure of the perfect, ordered surfaces of GaAs(110) and 2 × 1 Si(111) are similar, defects on the

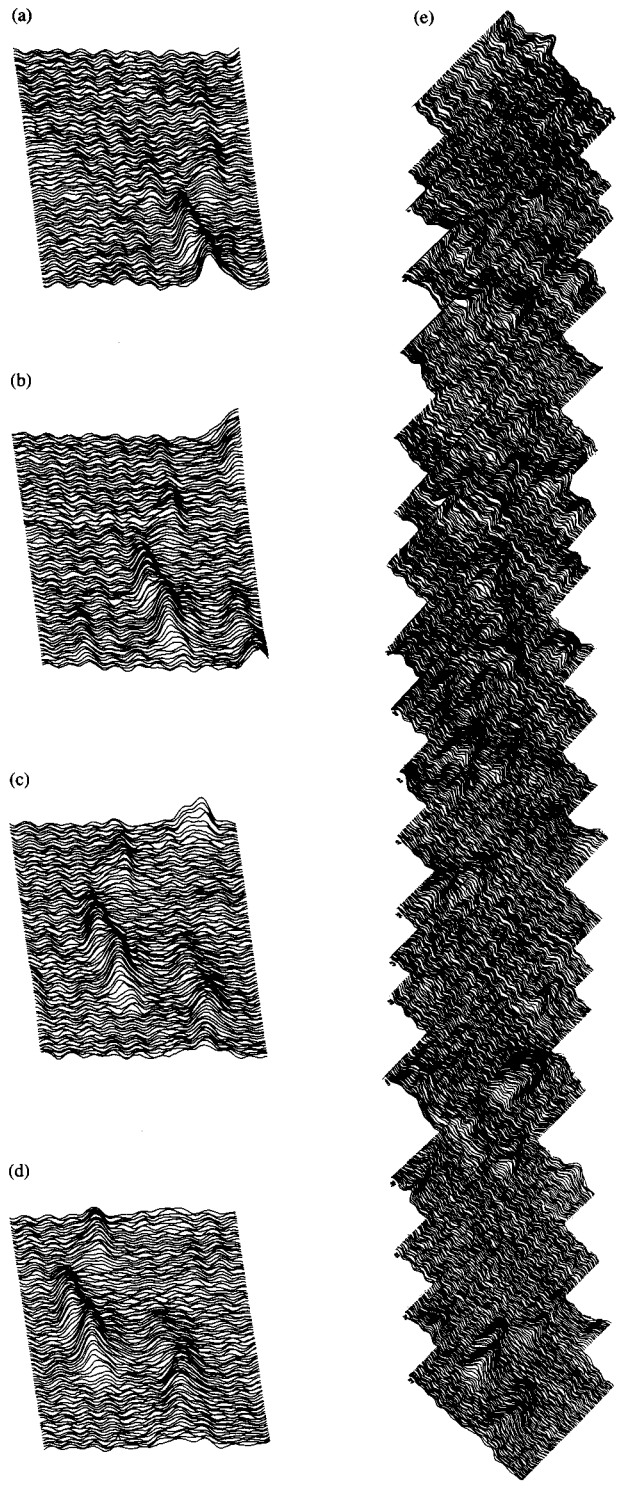

Figure 5

(a)–(d) Four successive STM images of Si(111), illustrating reproducibility of the images. The small lateral shift from one image to the next is due to drift of the STM. The relative scale of each image is the same as in Figure 4. (e) Overlay of a large sequence of images, extending over a lateral area of about 80 × 630 Å^2. Reprinted with permission from the *Journal of Vacuum Science and Technology.*

surface as observed by STM are quite different. On the GaAs surfaces we typically observe depressions ("holes") on the surface, indicative of missing atoms. Alternatively, on the Si surface the dominant structural defects are protrusions, indicating the presence of adatoms on the surface. This difference in the defect structure is not too surprising once we consider the surface structure in more detail. Although the atomic positions of the first two layers of GaAs(110) and 2 × 1 Si(111) are similar, the electronic surface structures in the two cases are quite different. In GaAs, electron transfer occurs between the Ga and As atoms, resulting in a rehybridization of the surface-atom bonds [4–6]. For Si, however, the dangling bond electrons are shared between the surface Si atoms, forming π-bonds [9]. This difference in electronic structure of the top atomic layer may affect the strength of the bonds connecting the top layer to the second layer. Below the second layer, the atomic structure of the two materials is, of course, completely different. Finally, it is important to remember that in the process of cleaving, the Si surface undergoes a significant reconstruction to form the 2 × 1 surface unit cells, whereas in the GaAs case the surface maintains 1 × 1 symmetry. This reconstruction of the Si surface may produce excess surface atoms which then act as adatoms, forming the protrusions observed here.

The difference in the surface bonds between GaAs(110) and 2 × 1 Si(111) produces a significantly different spectrum of surface states for these two materials. The Si surface has a large density of surface states within the bulk band gap [9], whereas the surface states of GaAs lie outside its bulk band gap [6, 14]. This difference is apparent in the voltages required to achieve stable tunneling currents. We have imaged the Si surface with voltages as low as 0.2 V, for which the tunneling current must be flowing through the surface states themselves. For GaAs, however, we generally have to use roughly 3 V to prevent contact between the tip and surface. These large voltages indicate the lack of a sufficient density of gap-states through which the current can pass.

5. Conclusions

In conclusion, we have used STM to study cleaved GaAs(110) and Si(111) surfaces. For the GaAs surface, we observe 1 × 1 surface periodicity and we find that common surface defects are small "holes" in the surface. On the Si surface we observe a periodicity of two unit cells indicating the 2 × 1 reconstruction. The amplitudes of the surface corrugations are consistent with the π-bonded chain model. The most common type of structural defect on the surface is "protrusions" along or crossing over between the chains. We also observe disorder in the asymmetry of the corrugation, indicating a tilt of the chains. The magnitude of the tilt varies, depending on the proximity of the chain to nearby structural defects.

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References

1. G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel, *Phys. Rev. Lett.* **50,** 120 (1983).
2. R. S. Becker, J. A. Golovchenko, and B. S. Swartzentruber, *Phys. Rev. Lett.* **54,** 2678 (1985).
3. R. M. Tromp, R. J. Hamers, and J. E. Demuth, *Phys. Rev. Lett.* **55,** 1303 (1985).
4. A. R. Lubinsky, C. B. Duke, B. W. Lee, and P. Mark, *Phys. Rev. Lett.* **36,** 1058 (1976).
5. R. J. Meyer, C. B. Duke, A. Paton, A. Kahn, E. So, J. L. Yeh, and P. Mark, *Phys. Rev. B* **19,** 5194 (1979).
6. S. Y. Tong, W. N. Mei, and G. Xu, *J. Vac. Sci. Technol. B* **2,** 393 (1984).
7. R. M. Feenstra and A. P. Fein, *Phys. Rev. B* **32,** 1394 (1985).
8. D. Haneman, *Phys. Rev.* **121,** 1093 (1961); *Adv. Phys.* **31,** 165 (1982).
9. K. C. Pandey, *Phys. Rev. Lett.* **47,** 1913 (1981); **49,** 223 (1982); *Proc. Indian Nat'l. Sci. Acad.* **51A,** 17 (1985).
10. F. J. Himpsel, P. M. Marcus, R. Tromp, I. P. Batra, M. R. Cook, F. Jona, and H. Liu, *Phys. Rev. B* **30,** 2257 (1984), and references contained therein.
11. R. M. Feenstra, W. A. Thompson, and A. P. Fein, *Phys. Rev. Lett.* **56,** 608 (1986).
12. N. J. DiNardo, J. E. Demuth, W. A. Thompson, and Ph. Avouris, *Phys. Rev. B* **31,** 4077 (1985).
13. G. Binnig and H. Rohrer, *Helv. Phys. Acta* **55,** 726 (1982); *Surf. Sci.* **126,** 236 (1983).
14. K. C. Pandey, J. L. Freeouf, and D. E. Eastman, *J. Vac. Sci. Technol.* **14,** 904 (1977).

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References

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3. R. M. Tromp, R. J. Hamers, and J. E. Demuth, *Phys. Rev. Lett.* **55,** 1303 (1985).
4. A. R. Lubinsky, C. B. Duke, B. W. Lee, and P. Mark, *Phys. Rev. Lett.* **36,** 1058 (1976).
5. R. J. Meyer, C. B. Duke, A. Paton, A. Kahn, E. So, J. L. Yeh, and P. Mark, *Phys. Rev. B* **19,** 5194 (1979).
6. S. Y. Tong, W. N. Mei, and G. Xu, *J. Vac. Sci. Technol. B* **2,** 393 (1984).
7. R. M. Feenstra and A. P. Fein, *Phys. Rev. B* **32,** 1394 (1985).
8. D. Haneman, *Phys. Rev.* **121,** 1093 (1961); *Adv. Phys.* **31,** 165 (1982).
9. K. C. Pandey, *Phys. Rev. Lett.* **47,** 1913 (1981); **49,** 223 (1982); *Proc. Indian Nat'l. Sci. Acad.* **51A,** 17 (1985).
10. F. J. Himpsel, P. M. Marcus, R. Tromp, I. P. Batra, M. R. Cook, F. Jona, and H. Liu, *Phys. Rev. B* **30,** 2257 (1984), and references contained therein.
11. R. M. Feenstra, W. A. Thompson, and A. P. Fein, *Phys. Rev. Lett.* **56,** 608 (1986).
12. N. J. DiNardo, J. E. Demuth, W. A. Thompson, and Ph. Avouris, *Phys. Rev. B* **31,** 4077 (1985).
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