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Surface morphology of GaAs(110) by scanning tunneling microscopy

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The surface morphology of cleaved GaAs(110) has been studied by scanning tunneling microscopy. Atomic rows (zigzag chains of alternating Ga and As atoms directed in the $[\bar{1}10]$ direction) are clearly resolved, and structure along the rows is also seen. The surface is observed to have 1×1 periodicity, with a [001] corrugation amplitude in the range 0.2–0.5 Å, and a $[\bar{1}10]$ corrugation amplitude of ~0.05 Å. Differences between images of *n*- and *p*-type GaAs are seen. Surface point defects are observed, consisting typically of 0.7-Å-deep depressions along an atomic row.

Scanning tunneling microscopy (STM) as developed by Binnig, Rohrer, Gerber, and Weibel[1,2] has proven to be a valuable technique for measuring surface morphology on an atomic scale. In this work, we report the first STM observations of topography of a *cleaved* surface, namely, GaAs(110). This surface has been extensively studied both experimentally and theoretically, and the purpose of this study is to find what additional features can be determined by STM, and also to see what can be learned about the technique of STM itself. 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, for example, in Ref. 3. 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.[3–5] This picture of the surface morphology as first determined by low-energy electron diffraction (LEED) is consistent with our STM results. In addition, we observe point defects on the surface in the form of 0.7-Å-deep depressions along an atomic row.

The tunneling microscope used in this study is similar to that described by Binnig *et al.*[1,2] Samples consisted of *n*-type (Si doped at 1×10^{18} cm^{-3}) and *p*-type (Zn doped at 3×10^{18} cm^{-3}) GaAs(100) wafers. These samples were cleaved *in situ* at a pressure of $<4\times10^{-11}$ Torr, exposing a (110) crystal face on the wafer edge. A constant tunneling current of 1 nA was used. The bias voltage between sample and probe tip was 3 V, with the sample at positive polarity for the *n*-type samples, and at negative polarity for the *p*-type samples. These relatively large bias voltages were required to prevent the probe tip from touching the surface, which generally occurred for biases of <1.5 V. Evaporated gold contacts of about 10 mm^2 in area were used on the wafers. Current/voltage measurements between two contacts indicated rectifying behavior with a zero-bias resistance of 20 kΩ, which is negligible compared to the tunnel-junction resistance. All of the STM images presented here consist of 100 data points along ≤100 line scans, with nominally 0.7-Å spacing between data points and line scans. A least-squares-fit planar background including a quadratic term in the *y* direction (perpendicular to the scan direction) has been subtracted from the images. In some cases, pairs of rows have been averaged to reduce hysteresis effects between opposite-direction scans. In general, thermal and piezo drift produce distortions in the images, so that, for example, atomic rows may appear slightly curved, or orthogonal lattice directions do not appear to be perpendicular in the image. Mechanically ground tungsten probe tips were used, with no special "tip-sharpening" procedure. These tips were not particularly stable, leading to abrupt *z*-level changes and/or resolution changes in the images.

The overall morphology of the cleaved GaAs surfaces consisted of atomically flat regions extending hundreds of angstroms laterally, separated by large steps. Isolated monatomic steps were rarely observed. In Fig. 1(a) we show an STM image obtained from an atomically flat region of *n*-type GaAs. The atomic rows directed in the $[\bar{1}10]$ direction are clearly seen. The lattice constant a_0 corresponds to the distance between rows, which is best measured by taking $1/\sqrt{2}$ times the wavelength along a given line scan (the crystal was mounted with the $[\bar{1}10]$ direction at 45° to the scan direction). We find a value of $a_0=6.0$ Å, compared to the accepted value of 5.65 Å. The difference between these values probably arises from a small calibration error.[6] The peak-to-valley corrugation amplitude measured from the image is about 0.5 Å. A numerical Fourier transform of the image is shown in Fig. 1(b) (the range of wave vector in this transform and in that of Fig. 2 is ±2.24 Å^{-1} for both k_x and k_y). The major peak with wave vector in the [001] direction is labeled (10). An orthogonal peak, labeled (01), is also seen, and referring back to the image one can see a faint structure along the atomic rows. In the transform, a relatively intense (11) peak is seen, along with a blurred (20) peak. The $(\bar{1}1)$ or $(1\bar{1})$ peaks are not seen, although they are probably obscured by the intense line at $k_x=0$, which arises from the discrete *z*-level changes (bands of lighter and darker topography) seen in the image. In Fig. 2(a) we show an STM image obtained from *p*-type GaAs. In this case the major corrugation with wave vector in the [001] direction is clearly visible, as is a smaller corrugation with wave vector in the $[\bar{1}10]$ direction. The peak-to-valley corrugation amplitudes measured from the image are 0.2 and ~0.05 Å, respectively. The resulting (10) and (01) peaks are indicated in the transform shown in Fig. 2(b). No (11) or equivalent peaks are seen. From the wavelength of the corrugations measured along a given line scan we deduce surface unit cell dimensions of 6.5×5.0 Å^2, which are fairly close to the accepted values of 5.65×4.00 Å^2 for 1×1 periodicity. The dark area near the center of the image is a surface point defect, and will be further discussed below.

Since the corrugation measured by STM is related to sur-

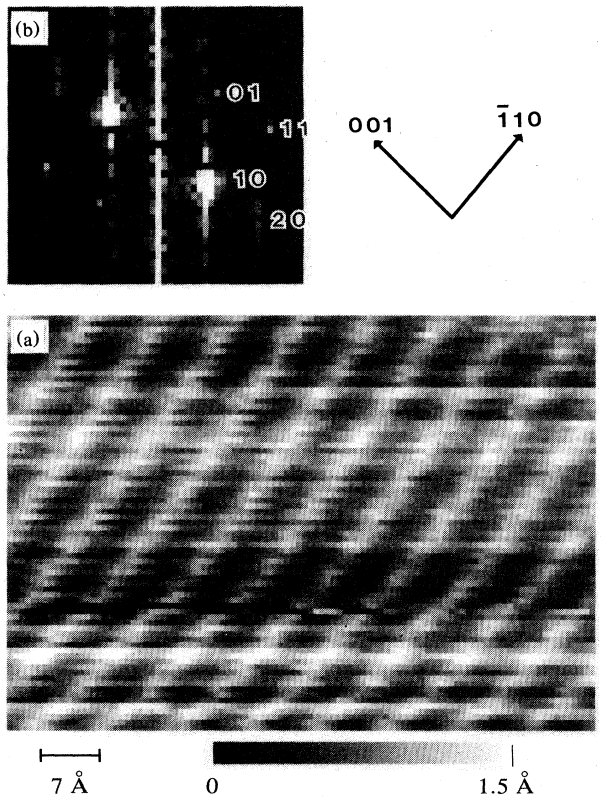

FIG. 1. (a) STM image of cleaved n-type GaAs(110); (b) a Fourier transform of the image. The image extends over an area of 70×53 Å^2, with surface height given by the gray scale ranging from 0 (black) to 1.5 Å (white). Atomic chains, with an actual lateral separation of 5.65 Å, give rise to the 0.5-Å vertical corrugation with wave vector in the [001] direction. This major corrugation results in the large peak labeled (10) in the transform. Smaller peaks in the transform are labeled accordingly.

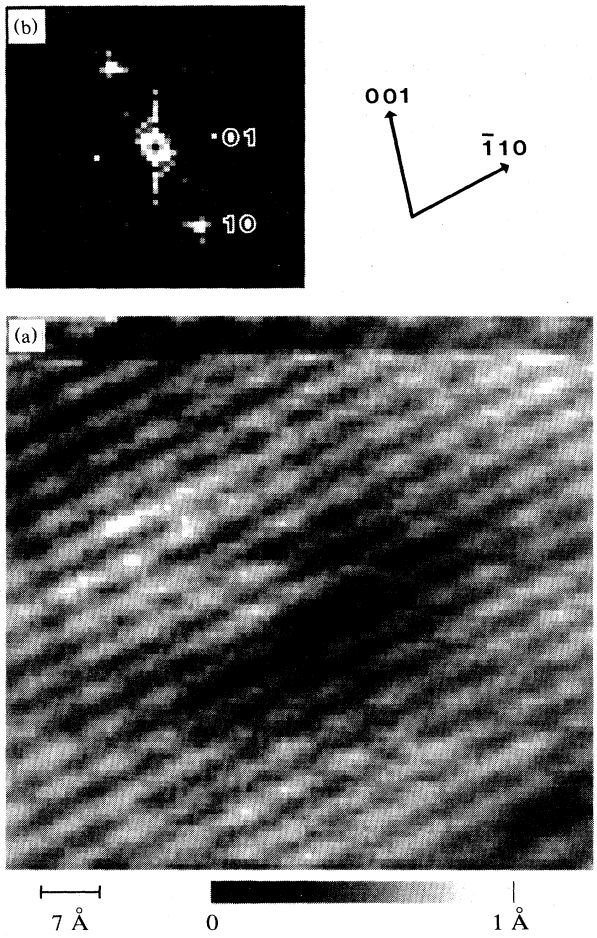

FIG. 2. (a) STM image of cleaved p-type GaAs(110); (b) a Fourier transform of the image. An [001] corrugation of 0.2 Å is seen in the image, along with a smaller [$\bar{1}$10] corrugation of ~ 0.05 Å. The lower (dark) region near the center of the image is a point defect.

face charge densities,[7] it is desirable to use STM to probe these charge densities. However, the observed corrugation depends on the precise atomic morphology at the end of the probe tip, which in our case is rather uncontrollable. Thus, we observe abrupt changes in resolution due to atomic rearrangements of the probe tip, as shown, for example, in Fig. 3(a). Furthermore, the resolution may not be circularly symmetric, as shown in Fig. 3(b), which is an image obtained from the same sample under the same conditions as that of Fig. 2(a). It is clearly evident that the ratio of minor to major corrugation is much less for Fig. 3(b) than for Fig. 2(a) [i.e., Fig. 3(b) shows very little structure along the atomic rows]. We note that the observed corrugations do not seem to depend on the scan direction, as demonstrated in Fig. 3(f), which was scanned in a direction perpendicular to that of Fig. 3(b), but which displays corrugations similar to those of Fig. 3(b). The images of Figs. 1 and 2 show the *maximum* observed corrugations. One interesting feature of these images is that the (11) peak is relatively intense for n-type GaAs and is not seen for p-type GaAs. This fact arises directly from the images in the following way: For p-type GaAs each unit cell appears as an isolated maximum in the topography, as shown in Fig. 2(a), and such maxima are composed primarily of (10) and (01) Fourier components. For n-type GaAs the atomic rows appear more as zigzag chains, as faintly seen in Fig. 1(a) (examine, for example, the structure along the atomic row originating in the upper-right-hand corner of the image), and such zigzag chains contain relatively large (11) Fourier components. This difference between n- and p-type images may be related to differences in the surface charge densities (neglecting band bending, the n-type image taken at positive sample polarity is sensitive to the conduction band, whereas the p-type image taken at negative sample polarity is sensitive to the valence band), although further work is required to confirm this result.

In addition to the 1×1 periodic structure seen in our STM images, we have observed defects on the surface. These defects are evident in Fig. 2(a) (near the center of the image and also seen at the lower-right corner) and also in Figs. 3(c), 3(d), and 3(e). The defects all look similar, consisting of a depression typically 0.7 Å deep 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

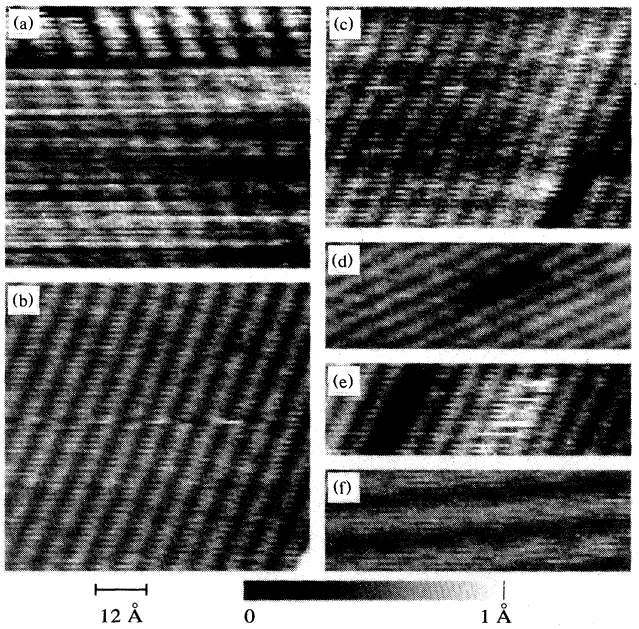

FIG. 3. Various STM images of cleaved GaAs(110): (a) illustrates a discrete resolution change during scanning; (b) and (f) are subsequent images with the x and y scan directions interchanged; (c)–(e) display surface point defects (dark areas).

rows are aligned both vertically and laterally on all sides of the depression, the defect is *not* a dislocation, but, rather, 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}). It is difficult to say at this point whether or not the observed defects are related to the Zn doping.

In summary, we have used STM to measure the surface morphology of cleaved GaAs(110). We observe 1×1 periodicity of the surface, in agreement with observations by other techniques. We observe a maximum corrugation of 0.5 Å, which can be compared with the atomic corrugation of the relaxed surface of about 2.1 Å (Ref. 4), and charge-density corrugation at the surface including both conduction and valence bands of about 2.0 Å (Ref. 7). Clearly one cannot directly obtain detailed geometrical quantities such as the Ga-As tilt angle directly from the STM images. Rather, the STM images provide a direct measure of surface charge densities near the Fermi level.[7] Also, STM yields local information about defects and disorder on the surface.

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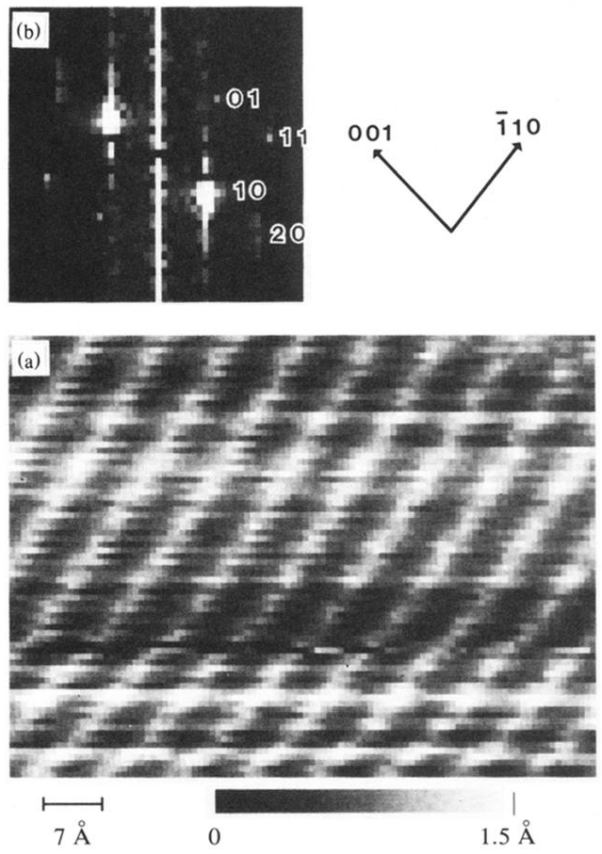


FIG. 1. (a) STM image of cleaved *n*-type GaAs(110); (b) a Fourier transform of the image. The image extends over an area of 70×53 Å^2, with surface height given by the gray scale ranging from 0 (black) to 1.5 Å (white). Atomic chains, with an actual lateral separation of 5.65 Å, give rise to the 0.5-Å vertical corrugation with wave vector in the [001] direction. This major corrugation results in the large peak labeled (10) in the transform. Smaller peaks in the transform are labeled accordingly.

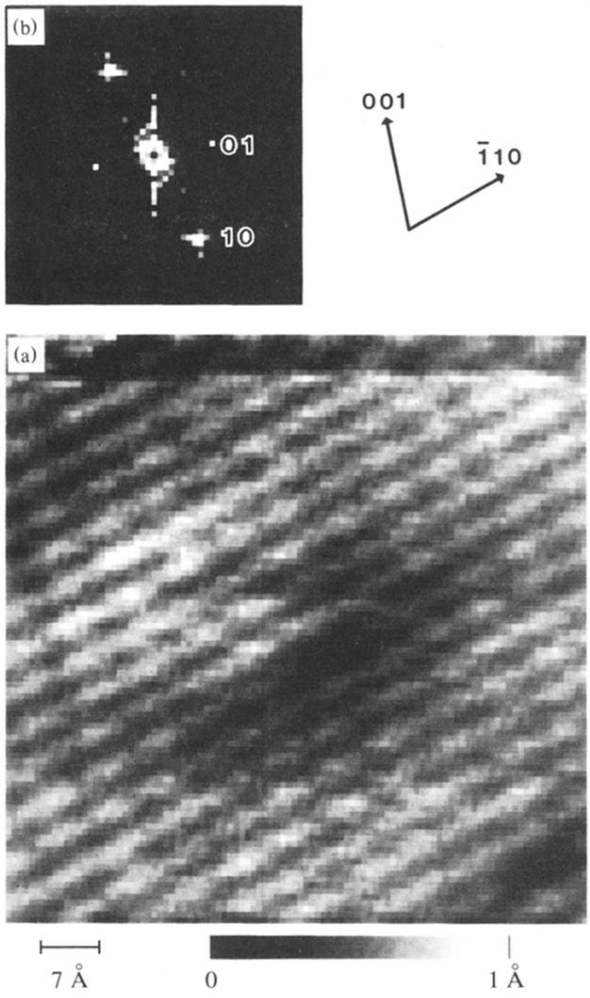
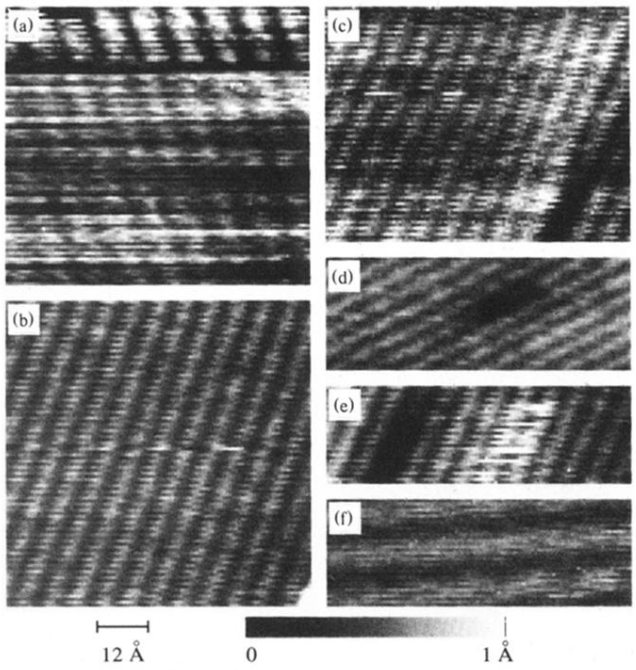


FIG. 2. (a) STM image of cleaved p-type GaAs(110); (b) a Fourier transform of the image. An [001] corrugation of 0.2 Å is seen in the image, along with a smaller [$\bar{1}$10] corrugation of ~ 0.05 Å. The lower (dark) region near the center of the image is a point defect.



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