Scanning Tunneling Microscopy of Crystal Dislocations in Gallium Arsenide

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Dislocations in GaAs induced by plastic deformation have been studied by scanning tunneling microscopy. Atomically resolved images of perfect and partial dislocations penetrating the cleaved {110} surface were obtained. A Burgers-vector analysis of the observed dislocations was performed. During observation the dislocations were found to be mobile over nm distances. No band bending was observed around the dislocation cores indicating that they are essentially electrically neutral.

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Scanning tunneling microscopy (STM) has proved to be a powerful tool for studying, on the atomic scale, the geometric and electronic structure of semiconductor surfaces. Up until now most of the work has concentrated on the investigation of ideal surfaces[1] and structural surface defects such as steps,[2,3] point defects,[4,5] surface reconstruction dislocations,[6] or domain boundaries.[7] In contrast, bulk crystal defects penetrating the surfaces have received little attention. Nevertheless, bulk defects such as grain boundaries accidentally penetrating the surface in the area studied have been seen and it was reported that dislocations induced by cleaving could be observed in the mineral galena (PbS).[8]

We report on a study of dislocations penetrating the {110} surface of plastically deformed gallium arsenide. The observations demonstrate the potential of STM to contribute to the understanding of bulk crystal lattice defects.

Feenstra and Fein were the first to obtain atomically resolved STM images of the {110} surface of cleaved GaAs.[9] This surface exhibits a simple 1×1 reconstruction. The electrons in the Ga dangling bonds transfer to the As atoms which move out of the surface plane by about 0.06 nm relative to the Ga atoms thereby shifting the surface electron states out of the band gap. Since the empty surface states are preferentially localized above Ga and the filled ones above the As atoms, the STM tip probes either atomic species separately depending on the sample bias voltage. Indeed, it was shown that the lateral position of the state-density maxima seen by STM correspond directly to the atomic positions of the Ga and As sublattices.[10] Because of this simple relationship between the STM images and the geometrical surface structure the {110} surface of GaAs is particularly suited for studying the structure of bulk lattice dislocations.

Samples with their long axis parallel to the [213] lattice direction were prepared from n-doped (10^{18} cm^{-3}) GaAs obtained from Wacker Chemitronic. They were deformed by 3.7% in compression at 400 °C under an argon atmosphere. Possible slip systems for the selected deformation geometry are $(\bar{1}1\bar{1})$ $[0\bar{1}\bar{1}]$ (primary system), $(\bar{1}1\bar{1})$ $[\bar{1}\bar{1}0]$, and $(1\bar{1}\bar{1})$ $[\bar{1}0\bar{1}]$ with Schmid factors 0.47, 0.35, and 0.29, respectively. The stress component acting on the primary slip system was 20 MPa. In order to avoid dislocation relaxation processes the stress was maintained during cooling the specimen to room temperature. The specimens were investigated by transmission electron microscopy (Philips EM430). The dislocation density was found to be about 10^8 cm^{-2}. Dislocations belonging to the two slip systems on the $(\bar{1}1\bar{1})$ plane were observed. The majority was of the screw type. However, 60° dislocations as well as edge dislocation dipoles were also found.

From the deformed samples rectangular specimens ($2\times3\times5$ mm^3) were cut with the long axis parallel to $[0\bar{1}\bar{1}]$. Figure 1 depicts the relationship between the sample geometry, the slip plane, as well as the relevant Burgers-vector and dislocation line directions. The slip plane is perpendicular to the surface and cuts it along

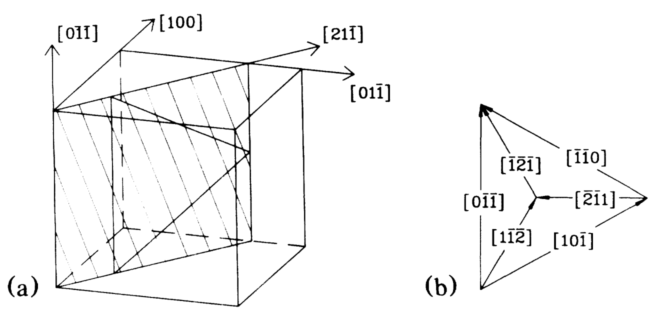


FIG. 1. (a) Relationship between the sample geometry and the $(\bar{1}1\bar{1})$ primary slip plane (hatched). The specimen surface normal is parallel to $[0\bar{1}\bar{1}]$. The orientation triangle in the slip plane is redrawn in (b). It marks the perfect and partial Burgers vectors as well as the dislocation line directions in the slip plane.

$[21\bar{1}]$. The primary Burgers-vector direction is parallel to the surface normal.

The samples were transferred into a UHV preparation chamber and cleaved along [100] by a double-wedge technique. Subsequently, the samples were transferred to the STM chamber via a UHV transfer system. The construction of the microscope is similar to a design developed by Besocke.[11] The sample holder rests on three piezoelectric tubes arranged in a triangular configuration. The scanner piezoelectric tube with the tungsten tip sits in the middle of the triangle formed by the outer tubes. To decouple the x-y motion of the tip from the z motion a small piezoelectric stack is mounted onto the scanner tube. Because of the highly symmetrical design the thermal drift is less than 1 nm/day. The lateral resolution of the microscope was calibrated by measurements on atomically resolved graphite. The z piezoelectric was calibrated by means of a laser heterodyne interferometer and measurements of step heights on GaAs. During cleavage and the STM observations the vacuum pressure was always below 10^{-8} Pa.

The following images were taken in the constant-current mode at sample voltages between -2 and -3 V and with sample currents between 1 and 2 nA. They therefore show the As sublattice. The images were median and linear filtered and not corrected for possible scan distortions. We found it difficult to obtain images with stable atomic resolution at positive sample voltages. This was presumably due to the presence of a GaAs-atom cluster on the tip deposited there in an accidental tip crash.

The following analyses of the dislocations are based on purely geometrical models of dislocations in the sphalerite structure.[12,13] At present it is too early to attempt to draw conclusions on possible quantitative modifications of these models from measurements of the exact position of the state-density maxima.

Figure 2 shows an image of an 11×11-nm^2 region showing the As-atom rows running parallel to the $[01\bar{1}]$ direction. The grey-scale variation along the [100] direction corresponds to a corrugation amplitude of about 0.03 nm. The atom separations along [100] are 0.56 nm. The core of a dislocation can be seen at C. The A step extends to the right parallel to $[21\bar{1}]$ where it crosses a monatomic cleavage step A-B. Regarding the picture at a glancing angle parallel to $[01\bar{1}]$, we find that close to the core the rows are bent with negative curvature below C and positive curvature above C. Furthermore, following the upper "bright" side of the step from left to right we notice that close to the core the atom rows are shifted upward. These shifts presumably result from surface relaxation under the action of the dislocation strain field.

Neglecting the described upward bending of the atom rows close to the core, we observe that the rows on the upper side of the dislocation-induced step are in line with the rows on the lower side. This indicates that the step

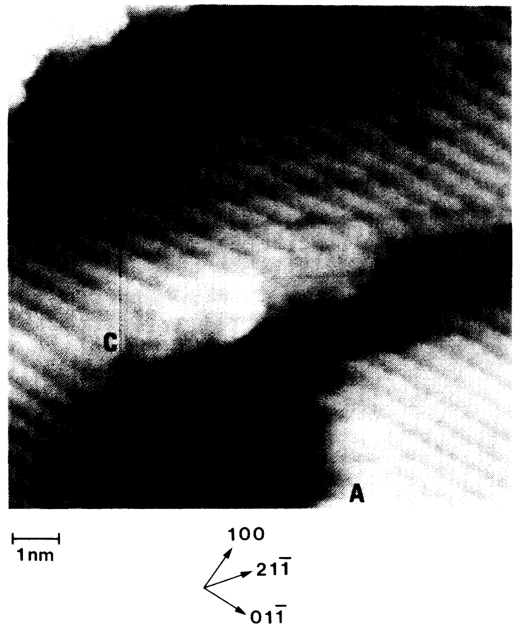
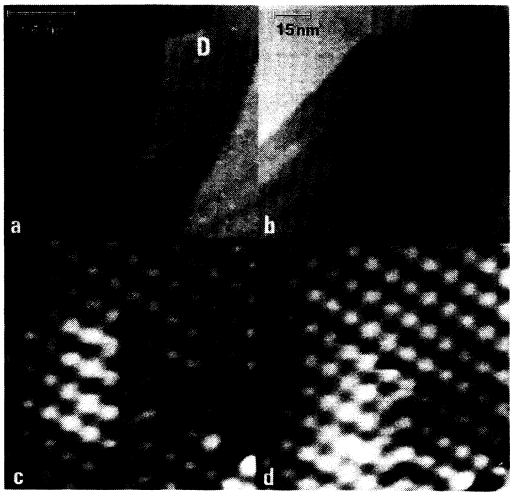


FIG. 2. Atomically resolved grey-scale image of a perfect dislocation with Burgers vector $\mathbf{b}=a/2[0\bar{1}\bar{1}]$ parallel to the surface normal producing a double atomic step on the surface.

comprises two atomic layers as was confirmed by measuring the elongation of the calibrated z piezoelectric. From this it can be concluded that the dislocation Burgers vector is parallel to the surface normal and of the form $\mathbf{b}=a/2[0\bar{1}\bar{1}]$, where a denotes the lattice parameter. The dislocation can be either a pure screw dislocation with the line direction $\boldsymbol{l}$ parallel to $[0\bar{1}\bar{1}]$ or a 60° dislocation with the line direction parallel to $[\bar{1}\bar{1}0]$ or $[10\bar{1}]$. Since there is no direct way to conclude the dislocation line direction from surface observations, we cannot distinguish between these configurations.

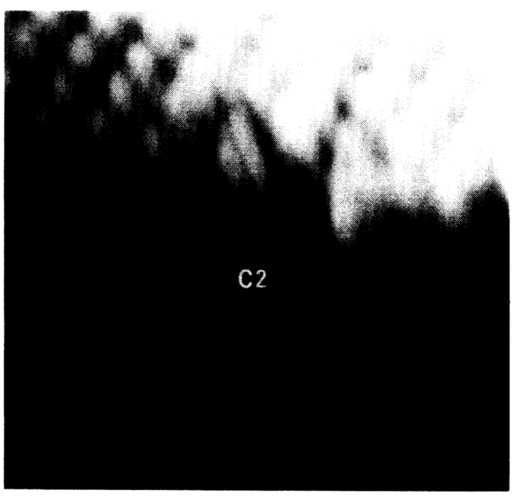
Figure 3 shows the two partials and the stacking fault of a dissociated dislocation. In Fig. 3(a) the core of the first partial appears as a depression at $C1$. The stacking fault extends along $[\bar{2}1\bar{1}]$. Following the As-atom rows along $[01\bar{1}]$, i.e., from the lower left corner to the upper right of the figure, we find that the rows on both sides of the stacking fault are not in line. The dislocation does not produce a step at the surface. From this it can be concluded that the Burgers vector is parallel to the surface plane and is given by $\mathbf{b}=a/6[\bar{2}1\bar{1}]$. On the upper right-hand side of Fig. 3(a) we note a point defect. Defects of this kind have been frequently observed on cleaved GaAs surfaces and were interpreted as As vacancies.[4]

In Fig. 3(b) the stacking fault of Fig. 3(a) can be seen again at the left-hand side. It ends in the core of a second partial dislocation at $C2$. From this dislocation a step runs along $[\bar{2}1\bar{1}]$ which, according to the step-height measurement, is monatomic. Following the atom rows across the step we find that they are bent at the upper



0.5nm $\bar{2}1\bar{1}$ $0\bar{1}1$ $\bar{1}00$

(a)



0.5nm $\bar{2}1\bar{1}$ $0\bar{1}1$ $\bar{1}00$

(b)

FIG. 3. The two partial dislocations and the enclosed stacking fault of a dissociated dislocation. The Burgers vector of the partial in (a) with core at $C1$ is $\mathbf{b}=a/6[\bar{2}1\bar{1}]$ and is parallel to the surface plane. As a consequence no surface step occurs. The Burgers vector of the second partial in (b) with core at $C2$ is $\mathbf{b}=a/6[\bar{1}\bar{1}\bar{2}]$. It produces a monatomic step running along $[\bar{2}1\bar{1}]$.

edge close to the core. Further away from the edge they are not in line with the rows in the lower part of the figure. These observations are consistent with a Burgers vector $\mathbf{b}=a/6[\bar{1}\bar{1}\bar{2}]$. This means that the total dislocation Burgers vector makes an angle of 30° with the surface plane and is given by

$$\mathbf{b}(\text{total})=a/6[\bar{2}1\bar{1}]+a/6[\bar{1}\bar{1}\bar{2}]=a/2[\bar{1}0\bar{1}]\,.$$

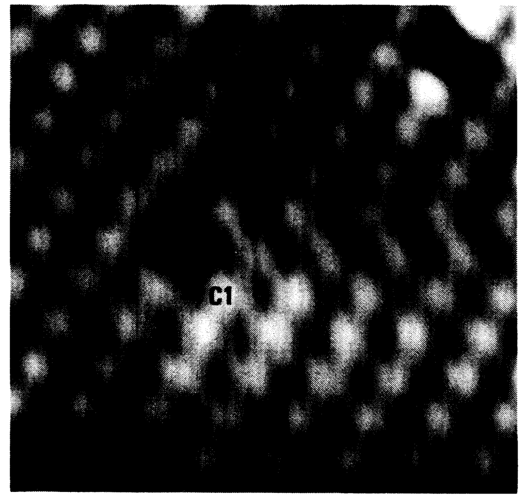


FIG. 4. Dislocation movement during STM observation. The dislocation marked by D in (a) has, after cross slip, reacted with a second dislocation in (b) forming a continuous step comprising two atomic layers. The core of the $C1$ dislocation of Fig. 3(a) is shown in (c). Two core images are seen since the core has moved downward during scanning. In (d) the core moves upward during scanning. The scan direction is from top to bottom.

The width of the stacking fault between the dislocations is about 12 nm. Again we cannot determine the dislocation line direction unambiguously. There are three possibilities: (i) 60° dislocation with $\mathbf{l}$ parallel to the surface normal $(0\bar{1}\bar{1})$; (ii) 60° dislocation with $\mathbf{l}$ at an angle of 60° to the surface normal; (iii) screw dislocation with $\mathbf{l}$ at 60° to the surface normal. In the first case, the first partial dislocation would be a 90° partial and the second a 30° partial. In the second case the reverse would hold. In the third case both partials would be of the 30° type.

The direction of the dissociation $[\bar{2}1\bar{1}]$ does not lie in the primary slip plane $(1\bar{1}\bar{1})$ but in $(11\bar{1})$. It is unlikely that any slip system in this plane was active during deformation since their Schmid factors are zero. However, the observations can be explained assuming that the dislocation is a screw dislocation which has cross slipped from the $(1\bar{1}\bar{1})$ plane containing the observed Burgers-vector direction $[\bar{1}0\bar{1}]$ onto the $(11\bar{1})$ plane.

An interesting phenomenon frequently observed is the movement of dislocations during STM observation. Figure 4(a) shows a low-magnification image of a dislocation at D. In Fig. 4(b) the dislocation has, after cross slip, reacted with a second dislocation forming a continuous surface step comprising two atomic layers. Figures 4(c) and 4(d) show the movement of the $C1$ partial dislocation of Fig. 3(a). While scanning horizontally from top to bottom the dislocation core in Fig. 4(c) moved from position 1 to position 2 at the time when the tunneling tip had just left the core area. As a consequence we obtain two core images. That this is not the result of a tip effect producing two images simultaneously can be seen from the unperturbed image of the As vacancy already mentioned above. It is known that under electron-tunneling conditions the forces locally exerted by the tip onto the surface atoms can reach values of about 10^{-9} N.[14] We therefore presume that the dislocation motion observed in our studies is a result of local stresses induced by the tip during scanning. Further work, however, should address the possibility of dislocation motion stimulated by charge-carrier injection and recombination.

During extended observation of the dissociated dislocation of Fig. 3 we observed the $C1$ partial frequently moving back and forth along the $[\bar{2}1\bar{1}]$ direction. However, the $C2$ partial remained sessile. This behavior can be explained on the basis of the difference in mobility of α and β dislocations in GaAs.[15] It has been reported in the literature that α dislocations are substantially more mobile than β dislocations.[16] This can be taken as an additional hint that the dislocation of Fig. 3 is of the screw type. Screw dislocations consist of an α and a β partial. On the other hand, 60° dislocations split in either all α or all β partial dislocations which would not allow us to explain the different behavior of the two partials observed here. We could indeed observe other dissociated dislocations with Burgers vectors consistent with 60° type where both partials moved simultaneously over large distances without changing their separation.

Varying the sample voltage between -4 and -1.5 V had little effect on the dislocation images. From this we can conclude that the observed dislocations are essentially electrically neutral. From the work on oxygen atoms on GaAs surfaces[17] and Ga vacancies on GaAs (Ref. 4) it is known that, due to surface band bending, the "images" of charged defects would be strongly dependent on bias voltage.

In summary, we have found that bulk crystal dislocations penetrating through the GaAs $\{110\}$ surface can be studied by STM on the atomic scale. The overall core structure of dissociated and undissociated dislocations can be compared to that of geometrical models describing bulk dislocations.[12,13] This is facilitated by the 1×1 reconstruction of the $\{110\}$ surface.

The current models of the core structure in the bulk are still incomplete. Recent high-resolution transmission electron microscopy[18] (HRTEM) of dissociated 60° dislocations yielded results which are in fair agreement with theoretical calculations[19] for the glide set configuration. However, instability of the dislocations under the electron beam and the possibility of jog formation (presumably facilitated by radiation damage) makes such observations difficult.

In HRTEM geometrical information on bulk crystal geometry is obtained by computer-assisted interpretation of dynamic interference patterns of transmitted electrons. In contrast, STM probes the local density of surface electron states. Therefore it primarily provides us with information on the electronic structure of dislocations at the surface. In order to be able to conclude in detail and quantitatively from the electronic structure on the geometrical structure at the surface and in the bulk a reliable theoretical link between the two is required. Although such details have still to be worked out, the present study has demonstrated the potential of STM for contributing to a better understanding of dislocations in GaAs and in semiconductors in general.

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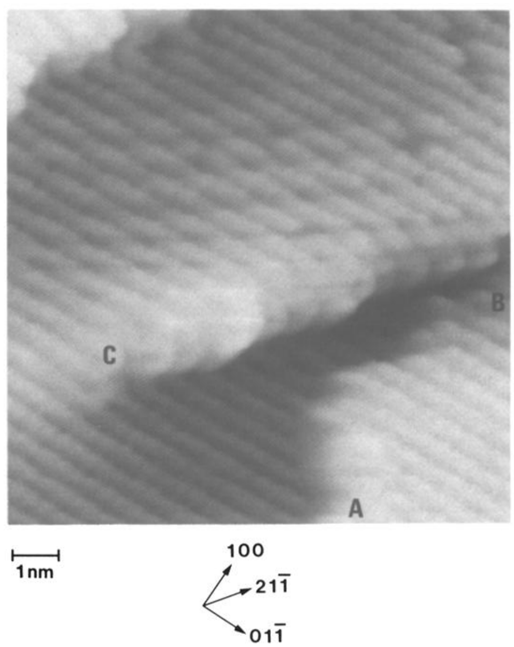

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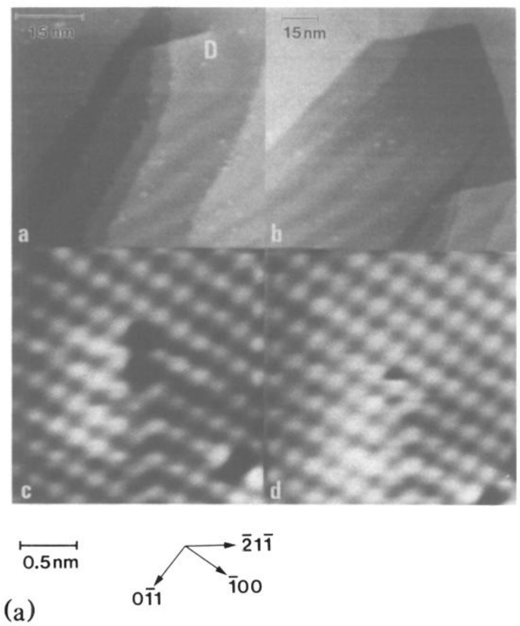
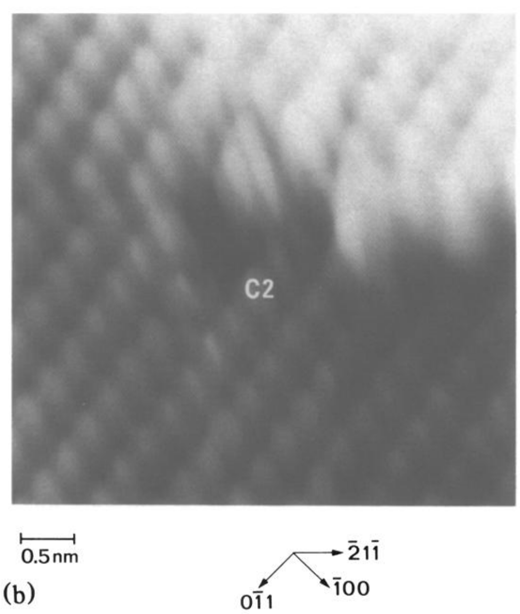
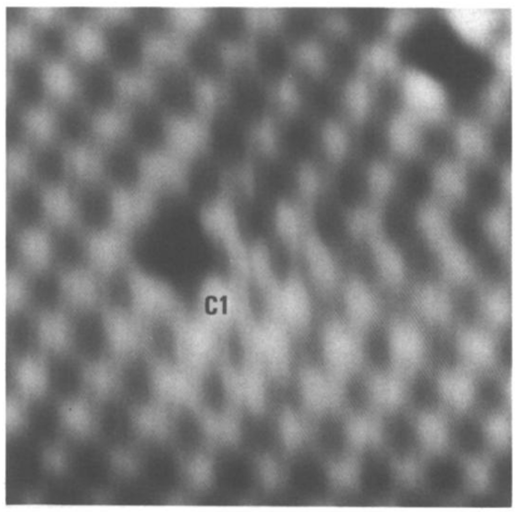


(a)



(b)

FIG. 3. The two partial dislocations and the enclosed stacking fault of a dissociated dislocation. The Burgers vector of the partial in (a) with core at $C1$ is $\mathbf{b}=a/6[\bar{2}1\bar{1}]$ and is parallel to the surface plane. As a consequence no surface step occurs. The Burgers vector of the second partial in (b) with core at $C2$ is $\mathbf{b}=a/6[\bar{1}\bar{1}\bar{2}]$. It produces a monatomic step running along $[\bar{2}1\bar{1}]$.



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