Z-contrast imaging of dislocation cores at the GaAs/Si interface

S. Lopatin[a)]
Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695

S. J. Pennycook
Oak Ridge National Laboratory, Solid State Division, P. O. Box 2008, Oak Ridge, Tennessee 37831

J. Narayan and G. Duscher[b)]
Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695

(Received 2 April 2002; accepted 13 August 2002)

The interface between silicon and epitaxial GaAs thin film grown by metalorganic chemical vapor deposition was studied using atomic-resolution *Z*-contrast imaging. *Z*-contrast imaging provides chemical composition information and allows direct interpretation of micrographs without simulation. Three different types of dislocations were identified. As expected, a dangling bond was found in the atomic structure of the 60° dislocation. One of the observed 90° dislocations had the reconstructed atomic core structure (with no dangling bonds). The core structure of the other 90° dislocation exhibited a dangling bond. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1511808]

One of the technological goals of the semiconductor industry is the monolithic integration of GaAs optoelectronic devices into high-speed silicon integrated circuits. By combining high-quality crystalline GaAs layers and silicon substrates, a wide variety of GaAs-based devices could be manufactured.[1]

Ideally, GaAs layers are grown heteroepitaxially on Si substrates. To avoid interdiffusion and reaction problems during the deposition of GaAs on silicon, a low-temperature process like molecular-beam epitaxy or metalorganic chemical vapor deposition (MOCVD) has been implemented.[2]

The major problem of manufacturing GaAs devices integrated in silicon technology is the lattice mismatch of 4.1% between GaAs and Si, which leads to the creation of a large number of interfacial dislocations (misfit dislocations). Dislocation densities of the order of 10^6 cm^{-2} are generally observed at the GaAs/Si interface. These dislocations may cause additional electronic states within the band gap that allow nonradiative recombination. Furthermore, impurities and other defects may be attracted to these dislocations, also forming nonradiative recombination centers. Therefore, dislocations may affect electronic and optical properties of the resulting GaAs based device.[3]

The majority of theoretical and experimental studies dealing with dislocations and critical thickness are based on diamondlike structures, because materials with these structures are most commonly used commercially. The dislocation with a Burgers vector of $\langle 110\rangle/2$ corresponds to the smallest primitive translation vector in such a system. These dislocations are called perfect dislocations.[4]

In the last few years, the dependence of interface dislocations on growth conditions and post growth treatment has been investigated extensively.[1,5–11] If the crystal growth direction is [001] and the dislocation line direction is $[1\bar{1}0]$, then Burgers vectors [101]/2 and $[01\bar{1}]/2$ both form a 60° angle with the dislocation line. These 60° dislocations originate from the steps of the free surface.[5] These two types of dislocations may react to form a dislocation with a Burgers vector of [110]/2, which is perpendicular to the dislocation line (90° dislocation).[6,7] The 90° dislocation may relieve the strain energy more efficiently than other dislocations because it is aligned with the strain–relaxation direction.

In this study, we used a dedicated scanning transmission electron microscope (STEM) for high-resolution *Z*-contrast imaging[12,13] of the 60° and 90° dislocations core structures at the GaAs/Si interface. The GaAs thin films were grown by MOCVD at 650 °C on a Si (001) substrate. Cross section $[1\bar{1}0]$ samples were prepared by standard mechanical polishing and ion milling.[14]

To obtain *Z*-contrast images, a crystalline sample is oriented to a low-order zone axis and scanned by the focused electron probe of the STEM. While the sample is scanned, an annular detector collects electrons scattered to high angles. Only 1*s* Bloch states reach the detector and contribute to the image,[15] achieving, in effect, column-by-column illumination of the crystal. The image is acquired serially, and represents a map showing the location of the projected atomic columns and their relative composition (high-angle scattering is proportional to the square of the mean atomic number *Z*). Thus, the structure of the crystal can be obtained directly from the *Z*-contrast image. We used a VG HB603 U dedicated STEM (300 keV, probe diameter less then 0.13 nm) to resolve individual atomic columns in Si or GaAs in the $[1\bar{1}0]$ direction so that the atomic structure of interfacial dislocations could be determined.

Figures 1(a)–3(a) show the *Z*-contrast images of a GaAs/Si interface with dislocations. The ellipselike bright spots are formed by two neighboring columns of Ga and As.

[a)]Electronic mail: slopati@unity.ncsu.edu
[b)]Also at: Oak Ridge National Laboratory, Solid State Division, P. O. Box 2008, Oak Ridge, TN 37831.

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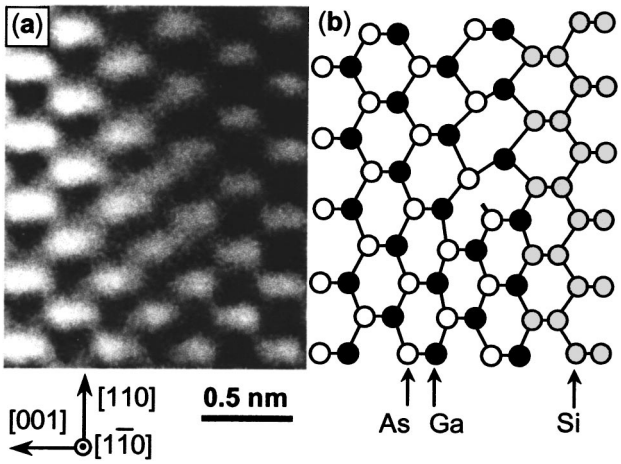

FIG. 1. Z-contrast image of a 60° dislocation (in $[1\bar{1}0]$) (a) and the structural model of the dislocation core (b). GaAs is heavier than Si and therefore appears brighter in the Z-contrast image.

The distance between such columns in $(1\bar{1}0)$ projection is 0.14 nm in GaAs (larger than the electron probe size), and should show as two circular spots that touch. However, these columns are not distinguishable in the vicinity of the dislocation core due to the stress fields caused by the dislocations. For the purpose of this study, this resolution degradation was not crucial because we were still able to distinguish between overlapping and single atomic columns. A single column shows nearly as a circle, whereas overlapping columns that are unresolved show as an ellipse. To confirm that a single atomic column was present, we also analyzed the intensity profiles of the columns in different directions. To determine the atomic species of the columns, we analyzed the intensity distribution along the [001] direction in the matrix far away from the interface ($\sim$10 nm) and thus established which side of the double spots had a lower ($Z_{Ga}=31$) or higher ($Z_{As}=33$) intensity. In this way, the relative position of Ga and As along GaAs layer and at the GaAs/Si interface was derived.

The number of 60° dislocations observed in this study was relatively small because most of them reacted to form 90° dislocations. Figure 1 presents a Z-contrast image of a 60° dislocation [Fig. 1(a)] and possible atomic model [Fig. 1(b)]. The dislocation core is compact and asymmetric. It forms an eight-sided polygon (octoring), consistent with the

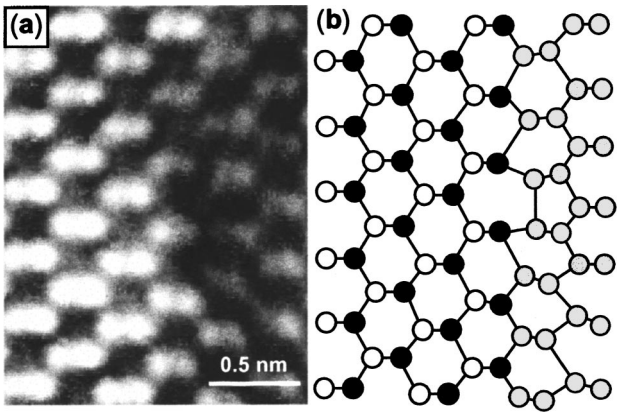

FIG. 2. Z-contrast image of a reconstructed 90° dislocation (in $[1\bar{1}0]$) (a) and the structural model of the dislocation core (b).

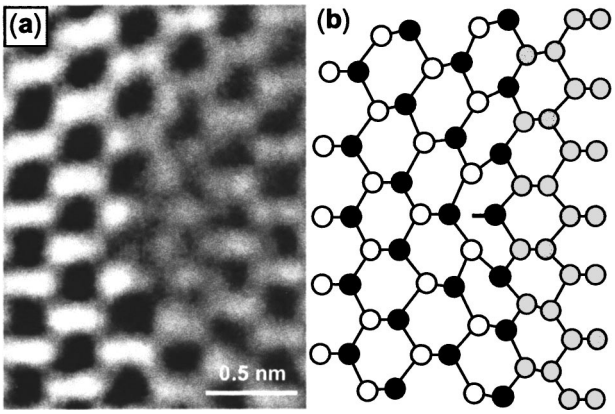

FIG. 3. Z-contrast image of nonreconstructed 90° dislocation (in $[1\bar{1}0]$) (a) and the structural model of the dislocation core (b).

expected structure for a 60° dislocation,[4,7,16] containing a single column of As atoms with a coordination different from the surrounding matrix. This constitutes a so-called dangling/broken bond, which is expected to cause additional energy levels in the band gap (midgap states).[3]

In contrast to the 60° dislocations, the 90° dislocations at the GaAs/Si interface showed a symmetrical configuration. Two different types of 90° dislocations were observed.

The reconstructed 90° dislocation is shown in Fig. 2. This dislocation causes even less distortion of the surrounding matrix than the 60° dislocations. In this configuration, there are no broken bonds and the well-known core structure consisting of five- and seven-fold ring units is observed.

Unexpectedly, we found another type of 90° dislocation. This 90° dislocation is not reconstructed but consists of structural units of six- and eight-fold rings (Fig. 3). A single atomic column is present at the center of the dislocation core, which causes dangling bonds. The presence of this additional column seems to be the reason for a strong stress field around the dislocation core. As a result, the position of neighboring atoms and the relative distance between them are different from those of the reconstructed dislocation [compare Figs. 2(b) and 3(b)].

Possible structures of 90° dislocations in diamond and diamondlike materials were discussed theoretically decades ago by Hornstra.[16] The following point was specifically stressed: Two types of 90° dislocations with [110]/2 Burgers vector and (001) glide plane may exist in diamond and diamondlike structures, and these two types can not simply be transformed into each other.

A single atomic column at the center of a dislocation core and the resulting dangling bonds are specific features of the nonreconstructed 90° dislocation (Fig. 3). A similar structure of threading dislocation was directly observed in GaN.[17] The reconstructed dislocation structure can be obtained from the nonreconstructed one by omitting the atoms with free bonds (Fig. 2). This reconstructed dislocation is known to exist in diamond and diamondlike materials. Its structure was calculated theoretically in Si and Ge.[18]

Although the presence of 90° and 60° dislocations at GaAs/Si interfaces was shown in recent years experimentally, the atomic structures of these dislocations were not investigated. It should be noted that the tendency toward reconstruction is relatively weak in GaAs.[11] This may be the

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reason that we found different dislocation core structures than those in Si or Ge.

Partial, dissociated, and Lomer dislocations were also reported at GaAs/Si interfaces.[9,10,19] It should be noted that in our Z-contrast images the stacking fault associated with dissociated dislocations could be clearly seen.[20] However, stacking faults were not observed in this study.

Therefore, both 60° and nonreconstructed 90° dislocations are associated with dangling bonds. In the case of 60° dislocations, the dangling bonds apparently originate from an As column [Fig. 1(b)], while in the case of the nonreconstructed 90° dislocations, the dangling bonds originate from an additional column which seems to be Ga [Fig. 3(b)]; this may introduce different energy levels in the band gap. Thus, one may expect different electronic properties for 60° and 90° dislocations, for example donor- versus acceptorlike behavior.[3]

In summary, Z-contrast imaging confirmed the existence of 60° and 90° dislocations at the GaAs/Si interface. Atomic structures of dislocations were obtained with a resolution high enough to distinguish a single atomic column of gallium or arsenic. As a result, this allowed us to observe the structure of nonreconstructed 90° dislocations with dangling bonds. Since both 60° and nonreconstructed 90° dislocations apparently exhibit dangling bonds, one may expect both types of dislocations to cause energy levels in the band gap, and therefore, to be detrimental to the electrical and optical properties of the GaAs/Si interface.

This work was funded by DOE-BES. The authors are grateful to M. F. Chisholm (Solid State Division/ ORNL) for enlightening discussions.

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