Direct observation of the core structures of threading dislocations in GaN

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Here we present the first direct observation of the atomic structure of threading dislocation cores in hexagonal GaN. Using atomic-resolution Z-contrast imaging, dislocations with edge character are found to exhibit an eight-fold ring core. The central column in the core of a pure edge dislocation has the same configuration as one row of dimers on the {10-10} surface. Following recent theoretical work, it is proposed that edge dislocations do not have deep defect states in the band gap, and do not contribute to cathodoluminescence dislocation contrast. On the other hand, both mixed and pure screw dislocations are found to have a full core, and full screw dislocation cores were calculated to have states in the gap. © *1998 American Institute of Physics.* [S0003-6951(98)02721-1]

Wide gap nitride semiconductors have attracted significant attention recently due to their promising performance as short-wavelength light emitting diodes (LED),[1] blue lasers,[2] and in other wide-ranging optoelectronic applications. One of the most intriguing issues concerning GaN is the fact that the material exhibits high-efficiency optical performance despite a density of structural defects which is six orders of magnitude higher than that for III-V arsenide and phosphide based LEDs.[3] The origin of these defects is well known and lies with the lack of a lattice- and thermal-matched substrate to GaN, meaning epitaxially grown hexagonal GaN films usually contain a high density of threading dislocations. These perfect dislocations with Burgers vectors of **a**, **c**, or **c+a** originate at the film/substrate interface and thread through the whole epilayer to the growth surface with line direction along ⟨0001⟩. However, the reason why the material is relatively insensitive to the presence of such a high density of these defects remains unclear.

In this regard, the results published in the literature present somewhat contradictory evidence. Cathodoluminescence (CL) studies have related the yellow luminescence centered at 2.2 eV to both threading dislocations at low angle grain boundaries[4] and to screw dislocations.[5] In addition, atomic force microscopy combined with CL imaging has shown that threading dislocations with a screw component (**c** or **c+a**) are nonradiative recombination sites.[6] Conversely, *ab initio* theoretical calculations show that both screw and edge dislocations are electrically inactive with no deep levels in the band gap.[7] However, in all of these cases a full interpretation of the results is hindered by the lack of knowledge concerning the precise atomic structure of the dislocation cores. The CL dislocation contrast may be due to the inherent dislocation core structure or impurity segregation around the dislocation,[8] and there is no experimental confirmation that the dislocation core structure assumed in the *ab initio* calculations is correct. It is therefore very important to know the exact configuration of the core structures from which an understanding of the optical properties can be developed. In this letter, we report the first direct observation of core structures of threading dislocations in GaN and discuss the results in light of the CL and *ab initio* results.

The GaN films used in this study were grown by metal-organic vapor phase epitaxy (MOVPE), a method which has been reported in detail in other papers.[9] However, a brief description of the growth process and general features of the film is presented here. The films were deposited on (0001) sapphire substrates in a low-pressure MOVPE reactor. The substrate was nitrided at high temperature before growth of a 2.6 nm buffer layer at 525 °C. By ramping the temperature to 1150 °C, growth proceeded under hydrogen with a V/III ratio of 1400. The dislocation density of the threading dislocations in these films is around 3×10^{10} cm^{-2}, with 68% pure edge, 30% mixed, and 2% pure screw dislocations, as determined by transmission electron microscopy.[10]

The core structures of these threading dislocations are studied here by high resolution Z-contrast imaging[11] in a 300 kV VG HB603 scanning transmission electron microscope with a resolution of 0.13 nm. Z-contrast microscopy is an incoherent imaging technique that differs significantly from

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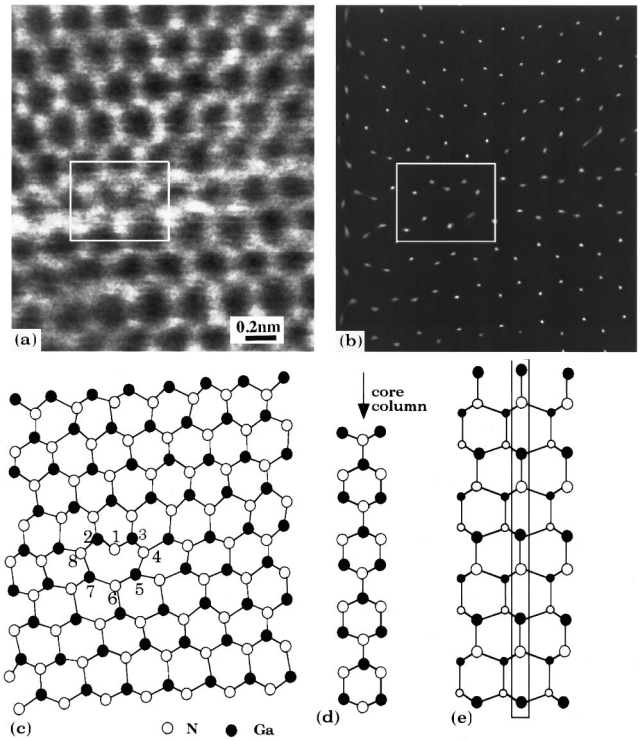

FIG. 1. (a) High-resolution Z-contrast image of a threading dislocation with edge character looking down ⟨0001⟩. The bright dots are atomic columns of alternating Ga and N atoms. The dislocation core is shown in the boxed region. (b) Maximum entropy image of Fig. 1(a) showing most probable column positions. (c) Sketch of the core structure determined from the experimental data. One double Ga–N layer is projected onto the c plane. Core columns are indicated by numbers 1 to 8. (d) Side view of the core structure of a pure edge dislocation projected onto the {10-10} plane showing similarity to one dimer row in the {10-10} surface in (e). Smaller symbols denoting the atoms below the surface.

conventional high resolution imaging in the mechanism of image formation. By detecting electrons scattered at high angles, individual atomic columns are imaged with a brightness that is proportional to their mean square atomic number (Z). As there are no contrast reversals, bright features always represent atomic columns and this permits an intuitive interpretation of the image intensity in terms of a core structure. Figure 1(a) shows a high resolution Z-contrast image of a threading dislocation viewed along ⟨0001⟩ GaN. Each bright spot is an atomic column comprising alternating Ga and N atoms. Figure 1(b) shows the maximum entropy[12] image of Fig. 1(a). As the Z-contrast image is a convolution of the probe intensity profile with the specimen object function, the maximum entropy routine allows us to recover the ''most likely'' object function, i.e., the specimen atomic structure, which is consistent with the image. Such an analysis allows the atomic positions of the columns to be determined within 0.02 nm.

Drawing the Burgers vector circuit around the dislocation determines that the core has an edge Burgers component of $\mathbf{b}=1/3\ [11\text{–}20]$. Clearly seen in the image are two extra {10-10} planes meeting at the core at an angle of 60° between them. The glide plane is {10-10}. It is obvious that the core structure is just an eight-fold ring, indicated by the numbers 1 to 8. Of the more than 20 individual cores analyzed, four were found to be pure screw dislocations, but *all* of the remainder showed the eight-fold core. This sample contained a mixture of edge and mixed dislocations (2:1), and so we conclude that all dislocations with edge character, both perfect edge and mixed dislocations, show the eight-fold ring structure in projection.

Figure 1(c) shows a sketch of the core structure projected along the ⟨0001⟩ direction, including just one Ga–N double layer. The structure we have determined for the perfect edge dislocation confirms the model proposed by previous theoretical calculations.[7] At the core, there is only one column having three-fold coordination, indicated as column 1. Figure 1(d) shows a side view of the atomic configurations of column 1 at the core of a pure edge dislocation, obtained by projecting the core onto the {10-10} plane, indicated by the arrow. Comparing with the structure of the {10-10} surface, this central column of the core is similar to a single row of dimers on the surface, as shown in Fig. 1(e). Unlike the Hornstra-core of a perfect edge dislocation in Si, which has five-fold and seven-fold rings, column 1 represents an extra column in the core of GaN, thus forming the eight-fold ring. It is reasonable that the core structure observed here has the lowest energy, because a Hornstra-like core in GaN would have Ga–Ga and N–N bonds. Even if columns 2 and 3 did not form such wrong bonds between them, the core would then have two rows of dimers equivalent to those in the central column of the eight-fold core. In both cases a higher energy would be expected, as reported by Elsner *et al.*[7] In their calculations, the eight-fold core was found to have the lowest energy, and relaxed in a manner identical to the {10-10} surface[13] by adopting a $sp^2(p^3)$ configuration.

To give an experimental estimation of the bond lengths, the distance between the core columns is measured from the image. The error bar for the measurement of the distance between columns is ± 0.02 nm, obtained from the statistics of the perfect regions in the original image. The distances between columns 7 and 8 and 5 and 4 are the same as the distance between undistorted columns within the error limit. The distances from column 6 to columns 5 and 7 are $15(\pm 10)\%$ *stretched*, while the distance from core column 1 to columns 2 and 3 is $15(\pm 10)\%$ *contracted*. These atomic positions are consistent with the theoretical calculations of the atomic displacements at the core.[7] Based on these calculations, therefore, the pure edge dislocation (which is charge neutral along the core) is not expected to have deep levels in the band gap of GaN. It is interesting to note that edge dislocations in AlN would be expected to have the same core structure of that in GaN. However, a recent calculation by Wright[14] does show edge dislocations to have deep defect states in this material, which are formed from a lone pair of electrons on the N atom in the core column resulting in the localized states at the dislocation core. The difference between GaN and AlN may probably be because of the much wider band gap (6.2 eV) and more ionic character of AlN.

Figure 2(a) shows a low magnification Z-contrast image in which dislocations are seen as bright dots, as a result of diffraction contrast from their strain fields. At high magnification, many of these dislocations showed the core structure seen in Fig. 1. Some, however, showed no disturbance to the lattice periodicity, as in Fig. 2(b), for example. Such dislocations have no edge component to their Burgers vector, and must therefore be pure screw dislocations with $\mathbf{b}=\pm\mathbf{c}$. As

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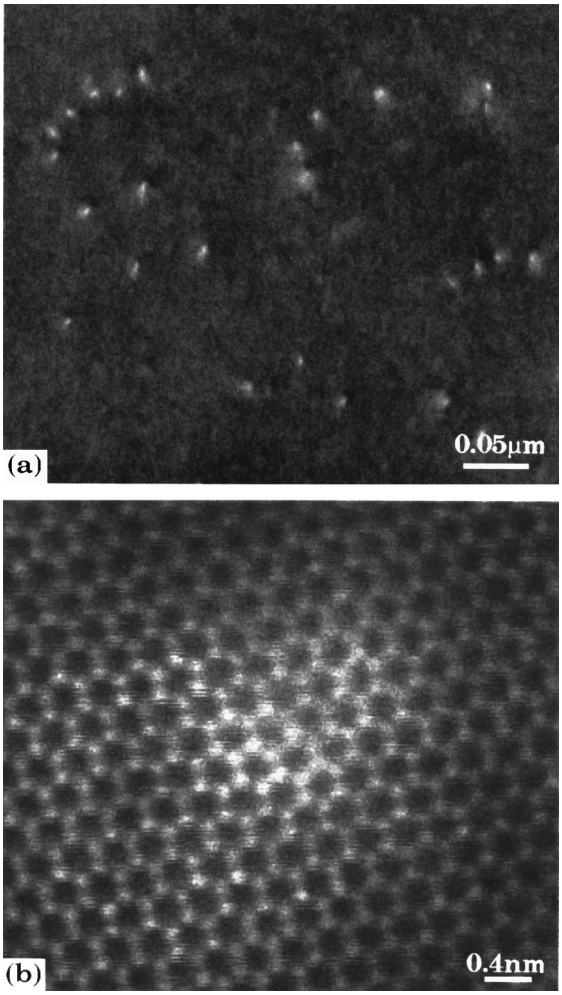

FIG. 2. (a) Low magnification annular dark field image along ⟨0001⟩. Threading dislocations show as bright dots due to their strain field. (b) High resolution *Z*-contrast image of an end-on pure screw dislocation showing a full core.

the dislocation is viewed end on, the displacement of the atoms due to the dislocation strain field cannot be seen. Although it is not possible from this image to locate the core exactly, it is obvious that this screw dislocation has a full core rather than an empty one. It is therefore important to note that screw dislocations can exist with both a full core as well as the open-core structure reported previously in GaN.[7,15] This is particularly important in the context of defect states in the band gap. As calculated by Elsner *et al.*,[7] full core screw dislocations have deep defect states in the band gap, presumably because of the larger bond distortions at the core. Similarly, we would expect that full core mixed dislocations, as we observe, would also have deep states in the gap because of similar distortions. Indeed, CL experiments confirm that both screw and mixed dislocations are related to nonradiative combination sites.[4–6] Based on these results it is expected that without impurity segregation, pure edge dislocations in GaN would not act as nonradiative combination centers, and would therefore be invisible in CL images.

In summary, the first direct observations of the atomic core structures of threading dislocations in GaN are presented. Core structures of dislocations with edge character, both pure edge, and mixed dislocations, are seen as eightfold rings in projection along their line direction. The central column in the core of a pure edge dislocation contains an alternating chain of Ga and N atoms similar to the structure of {10-10} surface dimers, confirming a recent theoretical prediction.[7] The pure edge dislocation is therefore not expected to have deep defect states in the band gap. However, full cores are found for pure screw dislocations and mixed dislocations. Based on the theoretical prediction that full core screw dislocations have defect levels in the gap, it is suggested that both screw and mixed dislocations have defect states in the band gap due to their screw components. This study provides a plausible explanation for the observed CL contrast at dislocations in GaN.

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