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A dissociation mechanism for the [a+c] dislocation in GaN

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Abstract. Mixed-type $[\mathbf{a}+\mathbf{c}]$ dislocations can be identified in atomic-resolution high-angle annular dark-field scanning transmission electron microscope images of GaN viewed along [0001] by use of a Burgers loop analysis and by observation of the depth-dependent displacements associated with the Eshelby twist. These dislocations are found to be able to dissociate resulting in a fault that lies perpendicular to the dislocation glide plane. Consideration of the bonding that occurs in such a fault allows the dissociation reaction to be proposed, and the proposed fault agrees with the experimental images when kinks are incorporated into the model.

1. Introduction

Despite the relatively high density of threading dislocations (with densities typically ranging from $10^7 - 10^9$ cm⁻²) that occur in GaN and its alloys because of growth on poor lattice-matched substrates, high-efficiencies can be achieved in blue emitting InGaN/GaN-based optoelectronic devices. The dislocations can, however, have a deleterious effects on lifetimes [1] and leakage currents [2,3] within these devices. It is known that the dislocations introduce electronic states into the band gap and act as non-radiative recombination centres [4,5]. Transmission electron microscopy (TEM) and scanning TEM (STEM) studies have been carried out to determine the core structure of these dislocations, with a recent publication noting the effect on core structures of Mg doping [6].

The general direction of these dislocations in (0001) oriented films is along [0001]. Three types of dislocations are generally found: edge-type dislocations with Burgers vector $\mathbf{b} = [\mathbf{a}]$, where \mathbf{a} is the unit cell lattice vector in the basal (0001) plane, screw dislocations with $\mathbf{b} = [\mathbf{c}]$, the unit cell translation along the [0001] axis, and mixed dislocations with $\mathbf{b} = [\mathbf{a} + \mathbf{c}]$. This paper presents highangle annular dark-field (HAADF) STEM images of the $[\mathbf{a} + \mathbf{c}]$ dislocation that show that a dissociation reaction can occur with this dislocation, and the proposed dissociation reaction and resulting fault are described.



2. Experimental details

Specimens of GaN (0001) layers grown on sapphire substrates, using the metalorganic chemical vapour deposition technique (MOCVD), were examined in an aberration corrected JEOL ARM 200F operating at 200 kV with a cold field emission gun. The 4.2 μ m thick GaN layer was undoped (not intentionally doped) and had a relatively low threading dislocation density of 4-5x10⁸ cm⁻². Plan view TEM samples were prepared using mechanical and ion polishing techniques.

3. Results and discussion

Figure 1 shows an image of a dislocation. It can be seen that the dislocation core appears to have a structure that is elongated with a fault parallel to the **a** plane (ie perpendicular to the **a** direction). The larger Burgers circuit shown in Fig 1(b) shows that the dislocation burgers vector has a component in the plane of the image of **a** and therefore it has an edge component. The atomic positions in the image do not, however, allow us to determine whether this dislocation has a screw component. A smaller circuit that encloses only one end of the fault shows a loop closure error of a/2, suggesting that the fault has been caused by a dissociation of the dislocation into partials. The Burgers loop analysis suggests that the edge component of the dislocation has dissociated by the following reaction

$$[\mathbf{a}] \rightarrow [\mathbf{a}/2] + [\mathbf{a}/2].$$

The glide plane (which must contain the **a** component of the Burgers vector and the dislocation line) is also marked on Fig. 1(b). It is clear that the dissociation has occurred in a direction perpendicular to the glide plane, and that therefore the edge component of the dislocation has dissociated in the climb direction.



Figure 1. (a) HAADF STEM images of a dislocation viewed end on along [0001] in GaN; (b) Burgers loops showing the edge component of the Burgers vector associated with the complete dislocation (yellow) and that associated with the defect at the end of the fault (green). The red line indicates the glide plane. The lattice vector **a** has a length of 0.319 nm.

We now turn to the possible structure of the planar fault caused by the dissociation. Figure 2(a) shows a model of a single layer of Ga and N atoms in one (0002) plane viewed along the [0001] direction. After removal of a line of atoms to create the a/2 displacement observed in the image, we find that the resultant fault consists of a large number of wrong bonds (Ga bonded to Ga and N bonded to N) that is likely to result in a high-energy fault and making dissociation unlikely (Fig 2b).



Figure 2. (a) a single (0002) plane of GaN; (b) removal of a line of atoms to give a shift by $\mathbf{a}/2$ resulting in wrong bonds; (c) a shift of the top part by $\mathbf{c}/2$ gives 4 and 8 membered rings with no wrong bonds.

The screw component offers a route to overcome this difficulty. Optical sectioning of the lattice surrounding this fault [7] shows depth-dependent displacements that are consistent with those expected to arise from the Eshelby twist. The Eshelby twist displacements [8] arise when a dislocation with a screw component intersects the free surfaces of the thin TEM sample, and their observation shows that the dislocation does have a screw component, which is likely be have a value of **c**, and the complete dislocation is therefore of the **a**+**c** type. If we make the assumption that the screw component of the dislocation dissociates through the following reaction

$$[\mathbf{c}] \rightarrow [\mathbf{c}/2] + [\mathbf{c}/2].$$

then the lattice on one side of the fault will be shifted by half a unit cell along the c-axis relative to the opposite side. Figure 2(c) shows that such a shift removes the wrong bonds, and results in a fault with alternating 8 and 4 membered rings but with no wrong bonds. Such a fault is likely to be relatively low in energy, as confirmed by numerical calculations and by considering the repulsion of the dislocations balancing the fault energy [9].

The projected structure of the fault (Fig. 2c) does not entirely correspond to the high resolution image of the fault seen in Fig. 3a. The 8 and 4 membered rings are marked in Fig. 3b, but additional atomic columns may also be seen. Optical sectioning focal series data of the dislocation [9] show that the dislocation is inclined at approximately 12° to the **c**-axis in a plane inclined to both the glide and climb planes. The dislocation must therefore contain both kinks and jogs along its length. Figure 3c shows the projected structure of the fault if we assume that there are two elementary kinks within the projected thickness of the sample. This shows better agreement with the experimental data. A more sophisticated analysis allows a more detailed model to be proposed [9].

Given that many more than two elementary kinks must exist along the dislocation within the thickness of the sample given the 12° inclination, the question then arises of why a reasonable agreement with the experimental image is achieved with only two kinks. The explanation is likely to be that the reduced depth of focus of the microscope only allows a thickness of sample to be imaged in high resolution in which approximately two kinks are contained given the 12° inclination, and indeed that it is the optical sectioning effect of aberration-corrected HAADF STEM that has allowed clear images of the fault to be achieved.



Figure 3. (a) The image from Fig. 1(a) reproduced with examples of the 8 and 4 membered rings highlighted. (b) A model containing two elementary kinks within the projected thickness gives better agreement with the image.

4. Conclusions

Mixed type $[\mathbf{a}+\mathbf{c}]$ dislocations can be identified in GaN viewed along [0001] by Burgers circuit analysis and by the use of optical sectioning to identify the presence of the screw dislocation. It is found that such mixed dislocation can dissociate, and the following dissociation reaction is proposed

$$[\mathbf{a}+\mathbf{c}] \rightarrow [\mathbf{a}/2+\mathbf{c}/2] + [\mathbf{a}/2+\mathbf{c}/2].$$

The resulting fault has the same structure as that observed by Drum [9] in AlN, and contains no wrong bonds. Agreement with the experimental images is made when the kinks associated with the inclination of the dislocation are included in the model.

5. References

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