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High-Resolution Z-Contrast Imaging

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DIRECT OBSERVATION OF THREADING DISLOCATIONS IN GaN BY HIGH RESOLUTION Z-CONTRAST IMAGING

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Wide gap nitride semiconductors have attracted significant attention recently due to their promising performance as short-wavelength light emitting diodes (LEDs) and blue lasers\textsuperscript{1}. One interesting issue concerning GaN is that the material is relatively insensitive to the presence of a density of dislocations which is six orders of magnitude higher than that for III-V arsenide and phosphide based LEDs. Although it is well known that these dislocations originate at the film-substrate interface during film growth, thread through the whole epilayer with line direction along \langle0001\rangle and are perfect dislocations with Burgers vectors of \(a\), \(c\), or \(c+\mathbf{a}\), the reason why they have such a small effect on the properties of GaN is unclear.

To develop a fundamental understanding of the properties of these dislocations, the core structures are studied here by high resolution Z-contrast imaging in a 300kV VG HB603 scanning transmission electron microscope (STEM) with a resolution of 0.13nm. Figure 1 shows a low magnification Z-contrast image of a plan view sample looking down \langle0001\rangle, in which dislocations are seen as bright dots (the brightness is a result of diffraction contrast from their strain fields). At higher magnification, the majority of dislocations are seen to be of edge character and have a core structure like the one shown in Figure 2a. As the Z-contrast image is a convolution between the probe intensity profile and the specimen object function, it is possible to obtain more detailed information on the specimen object function, i.e. the structure, through maximum entropy analysis (The maximum entropy technique produces the 'most likely' object function which is consistent with the image). As can be clearly seen in the maximum entropy image (figure 2b), the core structure is just an 8-fold ring, indicated by the numbers 1 to 8 in figure 2c. Comparing with the structure of the \{10-10\} surface, the central column of the core is similar to a single row of dimers on the surface, as shown in Figure 2d. Such a structure is not expected to have deep levels in the band gap and therefore should be electrically inactive\textsuperscript{2}.

Although the majority of dislocations had the above structure, some dislocations showed no disturbance to the lattice periodicity, as shown in figure 3. These dislocations have no edge component to their Burgers vector, and must therefore be pure screw dislocations with \(\mathbf{b} = \pm \mathbf{c}\). It is obvious from the image that this screw dislocation has a full core rather than an empty one. In this case, it seems likely that the larger bond distortions at these full core screw dislocations may lead to deep defect states in the band-gap. These observations provide the first direct experimental evidence of the atomic core structures of dislocations in GaN\textsuperscript{3}.

References:

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Fig. 1 Low magnification angular dark field image along \(<0001\). Threading dislocations show as bright dots due to their strain field.

Fig. 2 (a) High-resolution Z-contrast image of a threading edge dislocation looking down \(<0001\). (b) Maximum entropy image of Fig. 1(a) showing most probable column positions. (c) Sketch of the core structure determined from the experimental data. (d) Dislocation core showing similarity to one dimer row in the \{10-10\} surface. Smaller symbols denoting the atoms below the surface.

Fig. 3 High resolution Z-contrast image of an end-on pure screw dislocation showing a full core.