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ATOMIC STRUCTURES OF INVERSION DOMAIN BOUNDARIES AND DISLOCATIONS IN SINTERED ALN

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AlN is an attractive material because of its mechanical, thermal and electronic properties. However, these properties are often adversely altered by extended defects such as inversion domain boundaries (IDBs), and through impurities associated with the defects, especially oxygen. Thus to improve the properties of the material it is important to understand the structures of the defects. A number of studies have been carried out to characterize these defects using fringe contrast, weak-beam, convergent-beam electron diffraction and conventional high-resolution phase contrast imaging.¹⁻³ These techniques all require the use of model structures for data interpretation. In this paper, we report a direct determination of the structures of IDBs and dislocation cores in AlN by high-resolution Z-contrast imaging using a 300 kV VG HB603U scanning transmission electron microscope, with a probe size of 1.3 Å.

In sintered AlN, two types of IDBs are observed, a flat IDB lying on the (0001) basal plane and a curved IDB with no preferred habit plane. Fig. 1 shows a Z-contrast image of a flat IDB along [1120] zone axis and the projected structure derived from the image. The distance between an Al column and its nearest N column in the bulk in this projection is only 1.09 Å; hence they cannot be resolved, but the bright Al columns in the Z-contrast image clearly have an elongated shape due to the two closely spaced columns. From the presence of bright spots at the boundary it is immediately seen that the boundary terminates at the Al (0001) plane. These features are elongated more than in the bulk crystal, consistent with the presence of two adjacent N columns. The direction of elongation shows the arrangement of these two N columns. A schematic of the structure derived directly from the image is seen in Fig. 1(b). The dotted lines denote two unit cells in each domain, related by an inversion operation. The polarities of the two domains adjoining to the flat IDB have a head-to-head configuration, which is consistent with the result determined by CBED techniques⁵. It is known that flat IDBs are associated with oxygen impurities. Oxygen atoms may substitute for nitrogen atoms at the boundary to form a single octahedral Al-O layer. Our first-principles calculations confirm that this replacement causes an expansion at the boundary. This expansion is directly visible in the Z-contrast image. The expansion at the IDB is 0.3(±0.2) Å, consistent with the first-principles calculations.

The flat and curved IDBs often join to form dome-like defects. In this case, they are always connected by a dislocation. Fig. 2 shows the Z-contrast image of such a dislocation along [1120] zone axis. It is clearly seen that there is an extra (0001) plane at the dislocation. The core structure of the dislocation is deduced directly from the image.

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FIG. 1. (a) High-resolution Z-contrast image of a flat inversion domain boundary in sintered AlN. (b) the boundary structure derived from the image.

FIG. 2. High-resolution Z-contrast image of a dislocation core connecting a flat and a curved inversion domain boundary. The positions of inversion domain boundaries, the extra (0001) plane and the dislocation core structure are indicated.

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