The Atomic Structure of Threading Dislocations from Low-Angle to High-Angle Grain Boundaries in GaN/Sapphire Epitaxial Layers

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In GaN epitaxial layers, due to the mosaic growth mode, a large density of threading dislocations is present bounding misoriented grains ($\theta < 5^\circ$). Besides these low-angle grain boundaries, high-angle grain boundaries can be present as well. Here, we present an analysis of the $\Sigma = 7$ boundary using circuit mapping in order to define the Burgers vectors of the dislocations. In certain areas, the boundary is symmetric with the (2130) boundary plane. The periodic structure is comprised of an array of only one dislocation type. However, the cores of these dislocations possess more than one atomic configuration.

1. Introduction

The III–V nitride semiconductors are characterised by their large direct bandgap in the range 1.89 to 6.2 eV, which covers most of the visible spectrum and extends out into the ultraviolet range. GaN has been extensively studied and several technological breakthroughs have led to the commercialisation of high brightness light emitting diodes and laser diodes [1, 2].

These results are surprising if the large defect densities observed in the active layers are considered. The defects are mainly threading dislocations, basal and prismatic stacking faults, inversion domain boundaries and nanopipes [3 to 6]. Among them, we have focussed our attention on the threading dislocations which form high-angle grain boundaries. Adjacent crystals are rotated around [0001] and the interfaces can be described in terms of coincidence site lattices (CSL). CSL model is deduced by considering two identical interpenetrating lattices. If one lattice is rotated through a common lattice point, for certain angles, site lattices come into coincidence, forming the so-called coincidence lattice. $\Sigma$ corresponds to the ratio of the volume of the CSL unit cell and the primitive lattice.
2. Experimental Details

The GaN layers were grown on the (0001) sapphire surface by NH₃ gas source molecular beam epitaxy (MBE). The active layer was deposited at 800 °C on top of a low-temperature (550 °C) GaN buffer layer of 40 nm thickness. The plan-view samples were prepared as usual by mechanical grinding and ion milling. HREM experiments were carried out along the [0001] zone axis on a Topcon 002B electron microscope operating at 200 kV.

3. Crystallography

In the topological theory of line defects in interfaces developed by Pond [7], it was shown that all the admissible defects between crystallographically equivalent surfaces can be determined a-priori. In this formalism, one crystal is designated as white (λ) and the other as black (μ). The configuration formed by the interpenetrating lattices and crystals are called dichromatic pattern and complex, respectively [8]. The Burgers vectors of some admissible interfacial dislocations are given by:

\[ \mathbf{b}_{ij} = \mathbf{t}(\lambda)_j - Pt(\mu)_i, \]

where \( \mathbf{t}(\lambda)_j \) and \( \mathbf{t}(\mu)_i \) represent the \( i \)-th and \( j \)-th translation vectors in the \( \lambda \) and \( \mu \) crystals, respectively and \( P \) is a matrix which re-expresses \( \mathbf{t}(\mu)_i \) in the \( \lambda \) coordinate frame. The cores of such defects are associated with steps whose heights are given by \( h(\lambda) = n_\lambda \cdot \mathbf{t}(\lambda)_j \) and \( h(\mu) = n_\mu \cdot \mathbf{t}(\mu)_i \) where \( n \) are unit vectors normal to the interface, orientated towards the \( \lambda \) crystal.

These interfacial defects can be characterised in HREM images by circuit mapping as proposed by Pond [9]. A closed circuit is constructed on the micrograph with segments \( \mathbf{c}(\lambda) \) and \( \mathbf{c}(\mu) \) in the \( \lambda \) and \( \mu \) crystals, respectively. When the circuit is mapped into a reference space, any closure failure is equal to the total defect content and using the RH/FS convention, the defect is given by \( \mathbf{c}(\lambda,\mu)^{-1} \). If the circuit is mapped into a single crystal, the primary dislocations are exhibited, whereas in the dichromatic pattern, secondary dislocations are determined. In the simplest case, we obtain

\[ \mathbf{b}_{ij} = -\mathbf{c}(\lambda,\mu) = -\mathbf{c}(\lambda) - Pc(\mu). \]

4. Results

The GaN layers are made of mosaic grains rotated around the \( c \)-axis by angles in the range of zero to 20°. According to the value of the rotation angle \( \theta \), these boundaries can be classified as low-angle (\( \theta < 15^\circ \)) and high-angle grain boundaries (\( \theta > 15^\circ \)). The majority of the threading dislocations form low-angle grain boundaries. Burgers circuits drawn around the dislocations in these boundaries have given basal component for Burgers vectors equal to 1/3 \( (11\bar{2}0) \) (Fig. 1). The measured misorientation is \( \theta = 4.65^\circ \), in good agreement with the value calculated with Frank’s equation (\( \theta = 4.5^\circ \)). All the Burgers vectors were found to be perpendicular to the boundaries of the subgrain, these boundaries lying on the \{11\bar{2}0\} planes. The atomic structure of such dislocations has been previously studied and their cores were shown to be made of cycles with 8 or 5/7 atoms [10].
Besides these low-angle grain boundaries, high-angle grain boundaries are present [11]. We have studied a grain boundary with a rotation angle equal to 22° about [0001], very close to that of $\Sigma = 7$ misorientation in the CSL notation (21.79°). The grain boundary is facetted and the symmetric part in Fig. 2a corresponds to $(\overline{2310})_l/(1320)_m$. The large black dots define periods; by using circuit mapping around them, we deter-

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**Fig. 1.** Plan-view image, along the [0001] zone axis, showing a low-angle grain boundary. The dislocations are indicated by arrows.

**Fig. 2.** a) The periods of a high-angle symmetric grain boundary ($\Sigma = 7 : 21.79°/[0001]$) are shown by the large black dots. A circuit has been drawn and mapped in the $\lambda$ crystal. b) Reconstruction and c) simulation of the same boundary made of 5/7 and 8 atom cycles (thickness: 6 nm and defocus: −24 nm).
mined their dislocation content. We found for SXF: $c(\lambda) = SX = 1/3 [4150]_h$, and $c(\mu) = XF = 1/3 [5140]_h$. By reporting the circuit SXF in the $\mu$ crystal, the closure failure is $FS = a_2$, corresponding to one primary dislocation. When the same circuit is mapped into the dichromatic pattern rather than into the lattice of a single crystal, secondary dislocations may be determined. In this case, this leads to: $c(\lambda) + P_7c(\mu) = 0$. Therefore, in this period, the interface appears to be completely flat, without any additional defect. The result is exactly the same if circuits around the other periods are mapped.

The atomic structure of this grain boundary has been studied and the cores of the primary dislocations were found to contain 8 and 5/7 atom rings. In this area, there are five 5/7 core configurations followed by two 8 atom ring ones. A high resolution simulation of this boundary was carried out based on the reconstruction indicated on the experimental image and a good agreement was obtained for a thickness of 6 nm and a defocus value of $-24$ nm (Figs. 2b and c).

5. Conclusion

A $\Sigma = 7$ GaN grain boundary has been analysed using circuit mapping. In this boundary, we have identified the periodic structure of the $\Sigma = 7$ symmetric interface. Its atomic structure is based on several $1/3 \langle 1120 \rangle$ dislocation cores made of 5/7 and 8 atom cycles, as for the isolated threading dislocations.

References