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HREM study of stacking faults in GaN layers grown over sapphire substrate

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Abstract. Epitaxial GaN layers grown on sapphire contain a very large density of defects (threading dislocations, stacking faults, inversion domain boundaries, . . .). Among these defects, we have performed the analysis of the basal stacking faults by high resolution transmission electron microscopy. Two faults, I_1 and I_2, were identified. The formation of the I_1 fault is based on the climb-dissociation process of the $\frac{1}{3}\langle 11{-}20\rangle$ or of the [0001] perfect dislocations whereas the I_2 fault is due to the shear of the structure leading to a partial dislocation loop.

1. Introduction

Since the last decade, the III–V nitrides semiconductors have been extensively investigated because of their potential applications. This world wide research effort has led to optoelectronic devices operating from yellow to ultraviolet [1, 2]. However, problems still exist and are mostly due to the lack of suitable substrates. Until now, the best results were obtained for GaN layers grown by metallorganic chemical vapour deposition on the c-face of sapphire. The large mismatch, close to 16%, and the different thermal coefficients lead to the presence of densities of defects, up to five orders of magnitude higher than in conventional semiconductors [3]. One of the most surprising features of these materials is that devices may operate despite this high density of defects [4]. However, these defects influence the electronic and optical properties of the devices, particularly their efficiency and their lifetime [5]. Thus, in order to improve the quality of the layers, it is necessary to establish a connection between the presence of the defects and the properties of the devices, determining the structure and their formation mechanism.

In this work, we have focused our attention on the basal stacking faults. Their presence has been reported on sapphire and SiC substrates close to the interface, in GaN layers grown by molecular beam epitaxy or MOCVD, using an AlN buffer layer or not [3]. In bulk GaN grown under high nitrogen pressure, three types of stacking fault were observed (I_1, I_2 and E) whereas in GaN layers grown over sapphire, the presence of faults I_1 bounded by Frank–Shockley partials was reported [6–8]. An investigation of the electronic structure of stacking faults in GaN indicates that there are no defect-induced states in the band gap. However, stacking faults can give rise to quantum-well-like regions of zinc-blende materials embedded in the wurtzite lattice that can bind electrons [9]. This was confirmed by photoluminescence and transmission

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electron microscopy experiments that attribute an excitonic transition at 3.4 eV to the presence of stacking faults [10].

2. Crystallography

GaN occurs in two different polytypes (wurtzite and sphalerite) and the former is the more stable. The wurtzite structure consists of two interpenetrating hexagonal close-packed (hcp) lattices, related by the distance u along the c-axis ($u = 0.377$ for GaN); its space group is $P6_3mc$ (No 186). The wurtzite structure is related to hexagonal compounds in the same way as the sphalerite to the cubic ones. The difference between face-centred cubic and hexagonal close-packed lattices lies in the stacking sequence: AaBbCcAaBbCc… along the [111] direction and AaBbAaBb… along [0001], respectively. The capital letters correspond to cations and the lower case to anions (figure 1).

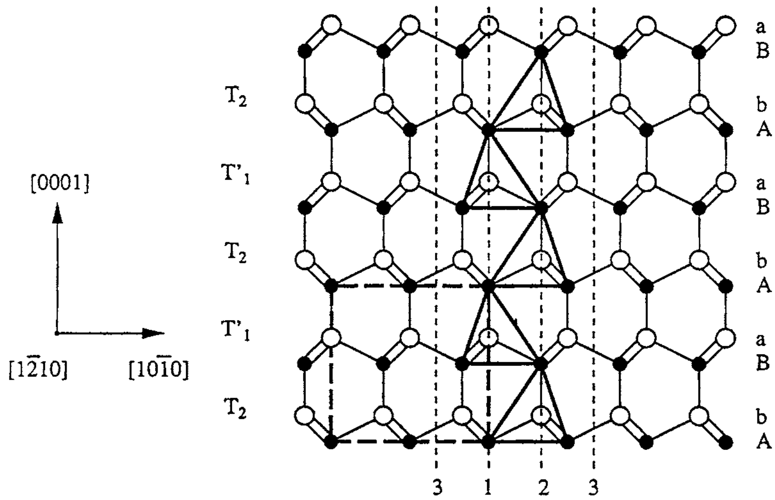


Figure 1. Wurtzite structure: projection along ⟨11−20⟩.

Basal stacking faults can be considered as errors in the usual stacking sequences, that preserve the original tetrahedral bonding. In the wurtzite structure, similarly to the hcp one, there are two kinds of intrinsic fault: I_1 and I_2 and one extrinsic fault E [11]. They correspond to one, two and three violations of the stacking rule, respectively. I_1 can be formed by the removal of one basal plane (for example Aa) followed by a shear of $\frac{1}{3}\langle 10-10\rangle$, shifting the Bb and Aa bilayers respectively to Cc and Bb. This leads to the following stacking sequence: AaBbAaBbCcBbCc…; the corresponding displacement vector is equal to $\frac{1}{6}\langle 20-23\rangle$ and the fault is bounded by Frank–Shockley partial dislocations. As the removal of a double layer is required, this type of basal fault cannot be obtained by the splitting of perfect dislocations into partials in response to deformation. However, it can be formed in wurtzite crystals during growth [12]. The fault I_2 can be formed directly by shear or after dissociation of a perfect dislocation $\boldsymbol{a} = \frac{1}{3}\langle 11-20\rangle$ in two Shockley partials. The stacking sequence of this fault is AaBbAaBbCcAaCcAa… and it is terminated by Shockley partial dislocations with Burgers vectors $\frac{1}{3}\langle 10-10\rangle$. The extrinsic fault E is formed by the insertion of a Cc bilayer, leading to AaBbAaCcBbAaBb…, the fault vector is $\frac{1}{2}[0001]$ and the fault is bounded by Frank partial dislocations (figure 2).

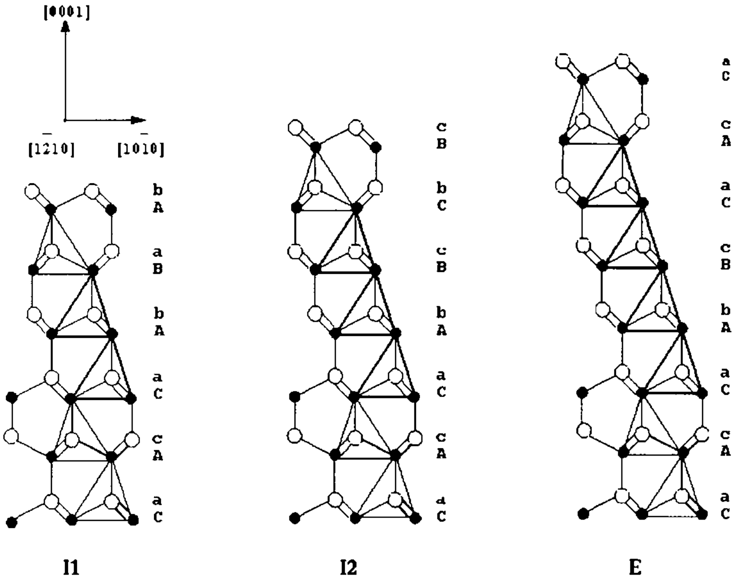


Figure 2. Intrinsic (I_1 and I_2) and extrinsic (E) stacking faults.

3. Experiment

The investigated GaN films were grown on a $3° \pm 0.5°$ misorientated (0001) sapphire substrate by MOCVD at 1000 °C. After nitridation of the substrate surface, a 15 nm GaN buffer layer was deposited at 500 °C. The samples for electron microscopy were prepared as usual by mechanical grinding and ion milling until electron transparency. HREM experiments were carried out along the [11–20] zone axis on a Topcon 002B microscope, operating at 200 kV, with a point to point resolution of 0.18 nm. HREM images were simulated using the electron microscopy software [13].

4. Results and discussion

In this paper, we present an analysis of basal stacking faults observed in the vicinity of the interface with the substrate.

At low magnification, we observed that a high density of defects is present near the interface, which are mostly dislocations and stacking faults. In the immediate vicinity of the sapphire substrate, the stacking faults extend to large distance, whereas far from it (20 nm) we mainly observed short width faults with an extension less than few tens of {10−10} lattice spacings. The large stacking faults are mainly I_1 and I_2, but segments of E fault were also observed [14]. In the following, we focus more particularly on the narrow basal stacking faults. Figure 3 shows a high-magnification image, along the ⟨11−20⟩ zone axis, of the GaN layer at 15 nm from the interface substrate. Two half {10−10} planes are underlined: they are separated by about ten lattice planes. By referring to the perfect wurtzite structure, the wrong stacking sequences can be underlined and we determined that these faults are I_2. These I_2 faults may occur following the dissociation of a perfect dislocation ($a = \frac{1}{3}\langle 11{-}20\rangle$) into two Shockley partials. However, the Burgers circuit drawn around these faults did not exhibit any closure failure. The two partial dislocations bounding these basal faults have opposite Burgers

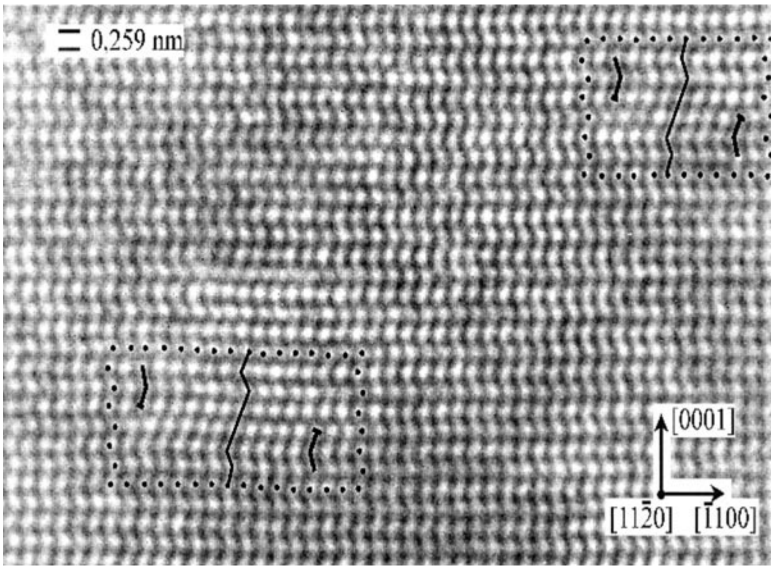


Figure 3. I_2 stacking fault associated with a partial dislocation loop.

vectors ($b = \frac{1}{3}\langle 10{-}10\rangle$). These faults I_2 can be formed directly by shear and we note that their presence is related to the end of the buffer layer.

Besides these I_2 faults, we show the existence of I_1 faults (figures 4(a) and (b)). In figure 4(a) an I_1 fault is present and the Burgers circuit drawn around shows a closure failure equal to $\frac{1}{2}\langle 10{-}10\rangle$ in the $\frac{1}{3}\langle 11{-}20\rangle$ projection. To the left of this fault additional (0002) and {10−10} half planes may be shown, whereas to its right is one half (0002) opposite plane. This I_1 fault corresponds to a climb dissociation of the perfect dislocation into two Frank–Shockley partials, following this reaction:

$$\tfrac{1}{3}\langle 11{-}20\rangle \rightarrow \tfrac{1}{6}\langle 20{-}23\rangle + \tfrac{1}{6}\langle 02{-}2{-}3\rangle$$

or

$$a \rightarrow (p_1 + c/2) + (p_2 - c/2)$$

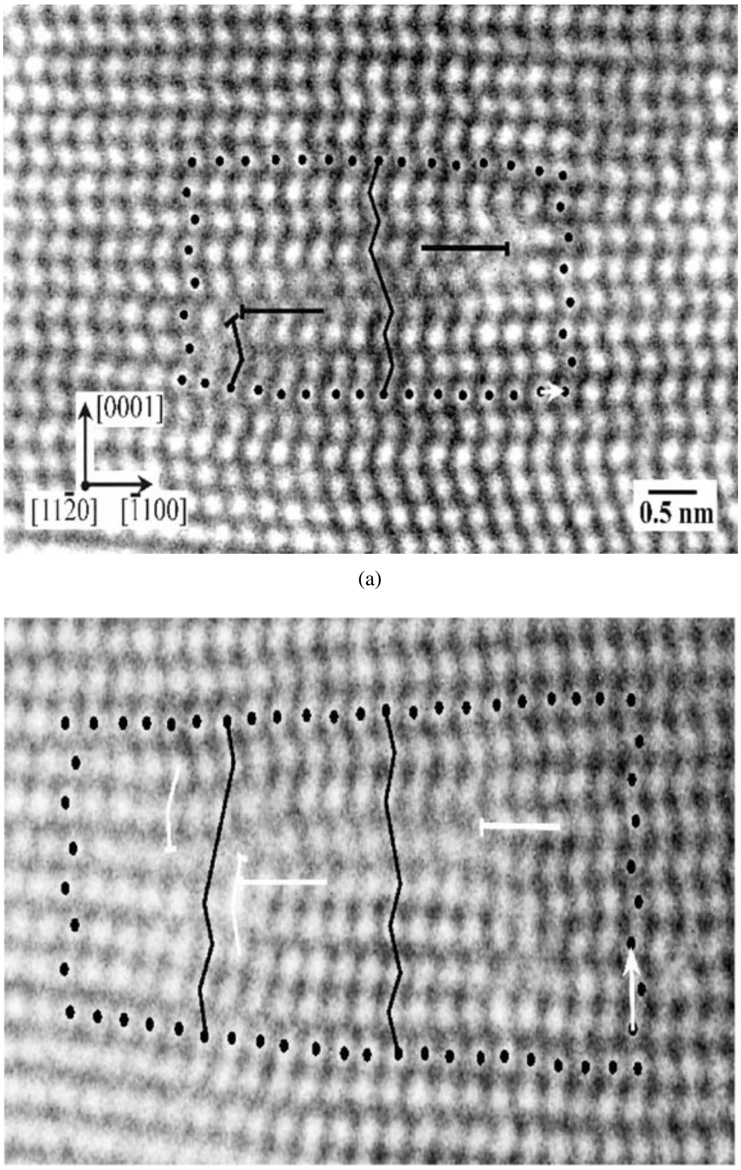
with p_1 the 90° partial and p_2 the 30° partial dislocations ($p_i = \frac{1}{3}\langle 10{-}10\rangle$).

Figure 4(b) shows two neighbouring basal stacking faults with a short extension, and when a Burgers circuit is drawn around them the closure failure appears to be equal to c. In fact, a careful examination indicates that there are two faults of I_1 and I_2 type. The I_2 is located at the left of the figure: it is bounded by two opposite partial dislocations ($b = \frac{1}{3}\langle 10{-}10\rangle$) like those presented in figure 3. Thus, it is not due to the dissociation of a dislocation but to a partial loop and does not contribute to the closure failure. On the right, an I_1 fault is present bounded by two Frank–Shockley partials; this fault results from a climb dissociation of a perfect $\boldsymbol{c}$ dislocation with

$$c \rightarrow (p_1 + c/2) + (-p_1 + c/2) \qquad \text{with } p_1 = \tfrac{1}{3}\langle 10{-}10\rangle.$$

As p_1 is a 30° partial dislocation no extra planes are visible, and only the two $\boldsymbol{c}/2$ partials contribute to the closure failure.

Previously, I_1 stacking faults were reported to exist in GaN layers grown on sapphire substrate by MOCVD [7, 8] whereas I_2 and E ones were not reported. In our case, we report the presence of both I_1 and I_2 faults close to the interface with the substrate. The fault I_1



(a)

(b)

Figure 4. (a) I_1 stacking fault due to the dissociation of an a dislocation bounded by two Frank–Shockley partials. (b) I_2 and I_1 stacking fault configuration, I_2 is a partial dislocation loop and I_1 is due to the dissociation of a c dislocation.

can be formed in wurtzite crystals during growth [11]. The fault I_2 can be formed directly by shear or after dissociation of a pure edge dislocation into two Shockley partials. The extended faults are observed in the first 15 nm of the GaN layer, which corresponds to the thickness of the buffer layer. It was previously shown that the buffer layer is predominantly cubic and transformed in hexagonal GaN during heating [15]. Thus, these faults may be due to incomplete transformation from sphalerite to wurtzite structures. Besides, the formation of the extended faults may be due to the mosaic growth mode of GaN/sapphire layers. The presence of steps, due to the 3° misorientation, can lead to the formation of defects as they create an additional shift between the epitaxial islands grown on adjacent terraces. The relaxation of the shift along [0001] is achieved by the insertion of stacking faults in the epitaxial layers [16].

Far from the interface, we observed I_2 faults with short extensions and the Burgers circuits drawn around them did not show up any closure failure. Thus, the small extended I_2 faults are not due to dissociations of perfect dislocations but to shear. They are observed at a thickness of 15 nm from the interface with the substrate and may be related to stresses associated with the termination of the buffer layer.

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