# A mechanism for the multiple atomic configurations of inversion domain boundaries in GaN layers grown on Si(111)

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Atomic structure investigation has been carried out on inversion domain boundaries in GaN layer grown on Si(111) by molecular-beam epitaxy. The comparison of the stacking sequences between simulated and experimental high resolution electron microscopy images shows the existence of two different atomic configurations for the inversion domain boundaries: the Holt model coexists with the V model inside the same layers. A mechanism allowing the switch from one model to the other by the interaction with the I1 stacking fault is proposed. © *2001 American Institute of Physics.*
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Ga-based III–V semiconductors nitrides are of great interest due to the possibilities they offer for optoelectronic devices[1] as well as high temperature and high power applications.[2,3] It was also recognized that GaN layers exhibit high efficiency luminescence even when containing a large density of extended defects.[4] The highest quality materials have been grown on either sapphire or silicon carbide substrate. The majority of GaN wurtzite films reported have the basal plane parallel to the substrate.[5,6] The availability of large, high quality wafers and the well known silicon technology make the silicon substrate an attractive alternative to silicon carbide and sapphire.

Direct growth of GaN on Si(111) is difficult due to poor nucleation, nevertheless improved GaN epitaxies have been obtained using an AlN or GaN buffer layer.[7–9] The optimization of AlN growth has been carried out using metalorganic chemical vapor deposition[10] and molecular-beam epitaxy (MBE).[11] Microstructural characterization of GaN over silicon substrates by transmission electron microscopy (TEM) has been performed for films grown by MBE.[12,13] The large mismatch with the silicon substrate results in the formation of different types of defects in the layer such as a high threading dislocation density.[13] Much work on high resolution electron microscopy (HREM) has been already devoted to characterize the inversion domains boundaries (IDBs) in GaN on sapphire substrates[14–17] in contrast to the GaN heteroepitaxy on Si(111) that has received less attention.

In the literature, several models have been developed in order to characterize the atomic structure of these boundaries. Initial geometrical models were proposed by Austerman and Gehman[18] and by Holt.[19] The IDBs model may be geometrically described in GaN using the changes in atomic positions at the interface, through an inversion operation and a translation. The Holt model is based on the exchange of the anion and cation sublattices leading to the formation of wrong bonds at the inversion boundary. Austerman and IDB* or V[16] models may be constructed from the Holt model by applying the suitable translation. A detailed description of these models has been carried out by Potin *et al.*[14–16] in the atomic structural characterization of IDBs in GaN films grown over sapphire. In spite of the presence of Ga–Ga or N–N wrong bonds, the Holt model explains the atomic structure in the IDBs observed by Potin *et al.*,[16] in contrast to the theoretical prediction.[20] Theoretically, IDB* or V model[16,17] with four and eight atoms rings in $[11\bar{2}0]$ projection has a lower formation energy in ionic-covalent materials, so the V model would be expected to be more stable in GaN.

In this work, the atomic structure of IDBs is studied in GaN grown by plasma-assisted MBE over (111)Si substrates on top of an AlN buffer in order to reduce the mismatch between GaN and Si(111). Experimental details of the growth can be found in Ref. 21. Cross section $\langle 11\bar{2}0\rangle$ TEM samples were prepared by mechanical grinding and dimpling down to 20 $\mu$m, followed by ion milling at 4.5 kV to electron transparency. HREM was carried out either on a TOPCON 002B electron microscope or on a JEOL 2000EX both operating at 200 kV. HREM image simulations were performed at different defocus and thickness values using the electron microscopy software (EMS).[22]

In the characterized specimen, different types of defects are present in the GaN epilayer. The GaN layer consists of a mosaic structure where the subgrains are slightly misoriented with a measured dislocation density of $1.4\times10^{10}\,\mathrm{cm}^{-2}$ reaching the GaN free surface. Stacking faults parallel to the basal plane and prismatic domains have been observed. For the later, the observed image contrast along polar axes is complementary, meaning that they are inversion domains.[23,24] Their size goes from 3 to more than 50 nm.[23]

HREM was performed on columnar domains, with the

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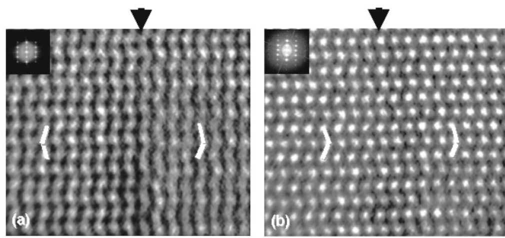


FIG. 1. Experimental images at (a) Scherzer and (b) −54 nm defocus of a V IDB are presented. (black arrows show the boundary).

orientation of the specimen along the $\langle 11\bar{2}0\rangle$ zone axis. Focal series were recorded around Scherzer and second contrast maximum (−54 nm), the fast Fourier transform (FFT) was calculated systematically for the analyzed boundaries in order to verify the defocus values. Figures 1(a) and 1(b) show the micrographs of an IDB recorded around Scherzer and second maximum contrast focus along with the respective calculated FFTs. As is clearly shown, at Scherzer focus, the AB stacking sequences are in opposite direction on both the right- and left-hand sides of the boundary. On the other hand, these AB sequences exhibit the same direction at −54 nm defocus [Fig. 1(b)]. Figures 2(a) and 2(b) correspond to HREM images of another boundary of the same specimen recorded under the same defocus values as in Fig. 1. As can be observed, the AB stacking sequence behavior in this area is completely opposite to the previous one. At Scherzer value focus, the AB sequences present the same sign, whereas at −54 nm the direction is different on both sides of the IDB.

As in the literature, image simulations allow one to distinguish between the atomic models of IDBs.[14–16] Simulations were carried out along the $\langle 11\bar{2}0\rangle$ zone axis, for defocus from 0 to −100 nm and thicknesses from 1 to 20 nm. For all the models, the AB sequence symmetry or asymmetry remains for thicknesses up to 20 nm. Through the comparison of experimental and simulated images, we concluded that the atomic model in Fig. 1 images corresponds to a V configuration, whereas Holt one is shown in Fig. 2. To our knowledge, the simultaneous occurrence of these configurations have not been previously reported on similar samples. Moreover, previous reports showed that the two configurations of IDBs formed independently in layers grown using different conditions, such layers exhibited very different and characteristic surface morphologies.[15]

Basal stacking faults can be considered as errors in the stacking sequence, making cubic GaN inclusions into the wurtzite matrix.[25] Basal stacking faults have been observed in GaN layers grown on sapphire and SiC substrates using different growth methods.[26–28] In bulk GaN, three types of stacking faults were observed ($I_1$, $I_2$, and $E$) whereas in GaN layers grown over sapphire, the presence of $I_1$ faults has been reported.[26,27,29]

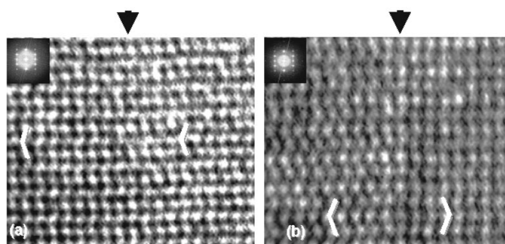
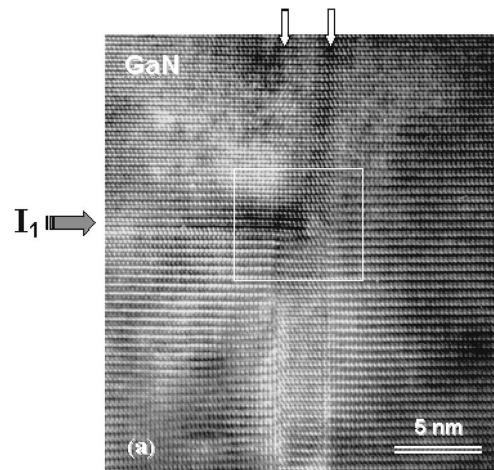


FIG. 2. Experimental images at (a) Scherzer and (b) −54 nm defocus of a Holt IDB are presented.



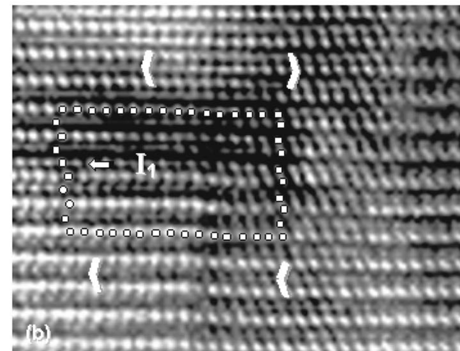




FIG. 3. HREM images taken along the $\langle 11\bar{2}0\rangle$ zone axis showing the interaction between an inversion domain and a basal stacking fault are presented. (a) A 3 nm wide inversion domain (vertical arrows) in which a $I_1$ stacking fault is incident (horizontal arrow) and (b) details of the interaction area: the ABC sequence of the $I_1$ stacking fault and the Burger circuit around the area are shown.

From the formation energy calculations[30,31] for the different basal stacking faults, it may be concluded that type $I_1$ possesses the lowest energy (10 meV/Å$^2$ in GaN), and therefore constitutes the most stable configuration. $I_1$ can be formed by the removal of a basal plane followed by a shear of $1/3\langle 0\bar{1}10\rangle$, its displacement vector is $R_{I1}=1/6\langle 0\bar{2}23\rangle$.[32]

As can be seen in Fig. 3(a), an $I_1$ stacking fault arrives into an inversion domain and does not cross it, however, the inversion domain continues without any visible modification towards the layer surface. When stopped, the I1 stacking fault is terminated by a Schockley partial dislocation:

$$1/6\langle 02\bar{2}3\rangle = 1/3[01\bar{1}0] + 1/2[0001].$$

In this case, only the modification of the stacking sequence is visible but there is no additional $c/2$ plane visible, meaning that this component of the Schockley partial has been absorbed by the IDB. Moreover, the Burgers circuit drawn around the area where it terminates the I1 fault does not show any closure feature [Fig. 3(b)] even in the basal plane, therefore the $1/3\langle 0\bar{1}10\rangle$ component lies at 30° from the $\langle 11\bar{2}0\rangle$ observation zone axis and is not visible.[33]

A possible mechanism, which can explain the aforementioned observations, is sketched in Fig. 4. From the left-hand side, an I1 fault arrives into the IDB which initially bears the

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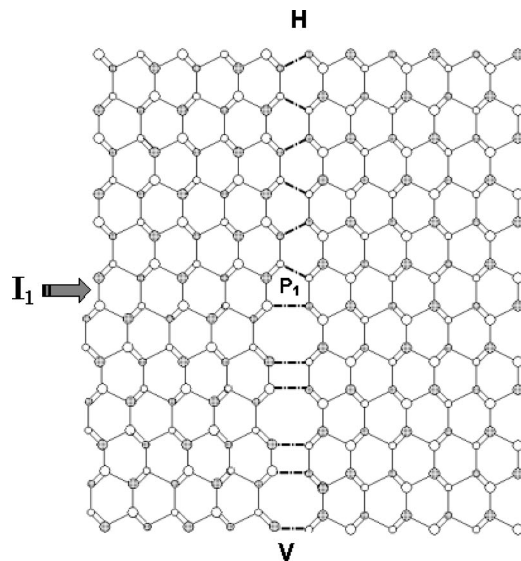


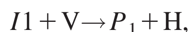


FIG. 4. Shematic drawing of the observed interaction mechanism between the inversion domain and a basal stacking fault is shown. $I_1$ and $p_1$ indicate the stacking fault and partial dislocation core, respectively.

V atomic configuration with the eight and four alternating atom rings. In the intersecting plane, the basal stacking fault terminates. The termination of the stacking fault issues a $c/2$ translation with switches the IDB from the V atomic configuration to a Holt one, with Ga–Ga and N–N wrong bonds. This may be formulated as follows:

$$I1 + \mathrm{V} \rightarrow P_1 + \mathrm{H},$$

where $p_1$ corresponds to the $1/3\langle 0\bar{1}10\rangle$ partial dislocation at 30° from the observation zone axis, explaining why no additional lattice planes are visible at the stacking fault termination point.

For the last few years, it has been argued that due to energetic factors, the only atomic configuration of the $\{10\bar{1}0\}$ IDB would need to be reconstructed in order to avoid the formation of Ga–Ga and N–N bond inside the III-nitride ionic semiconductors.[20] However, in our previous reports, it was shown that the Holt and the reconstructed atomic configuration could form, but these observations had been carried out in GaN layers grown in different epitaxial conditions.[14,16] The Holt configuration was shown to be in very small domains (~20 nm) inside layers having a flat surface, whereas the V one bordered larger domains (>50 nm) which terminated in the center of small pyramids which leads to a typical surface roughness for the layers.[15] These domains were shown to form only in nitrogen polar GaN layers.[34] The difference in their size was tentatively explained[35] on the basis of the *ab initio* calculations which indicate that the Holt-type configuration has a high formation energy.[20]

In this letter, it is shown that the two atomic configurations of IDBs in GaN can coexist inside the same layer. The analyzed layers contain domains of various widths, probably explaining the simultaneous occurrence of both configurations. However, it is also shown that it would be possible to switch from one configuration to the other by interacting with a basal stacking fault which has a $c/2$ component. In that case, it appears that only geometrical factors are acting, and probably, at the high growth temperatures, the kinetics of the growth dominates the other possible limiting factors.

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