Basal-plane Stacking Faults in Non-polar GaN Studied by Off-axis Electron Holography

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Abstract. We have studied basal-plane stacking faults in a non-polar (11-20) GaN epilayer using high-resolution electron microscopy and off-axis electron holography. The microstructure of the basal-plane stacking faults (BSFs) has been determined to be I1 type from high-resolution TEM images. High-resolution holograms along the [11-20] zone axis were obtained by off-axis electron holography on a Cs-corrected TEM, providing ∼2 Å spatial resolution in the reconstructed amplitude and phase images. Phase fluctuations across the stacking faults were detected, suggesting the presence of a built-in electric field. The uncertainties in the experiments and their interpretation are discussed.

1. Introduction
Gallium nitride based materials and structures are conventionally grown along the polar crystallographic c-axis. The spontaneous and piezoelectric polarization in this direction generates internal electric fields, which lower the radiative recombination efficiency in the quantum well (QW) structures. The growth of non-polar structures on α-plane (11-20) GaN eliminates the electric fields across the QWs, but the thin films generally have more defects such as basal-plane stacking faults (BSFs), prismatic stacking faults (PSFs) and partial dislocations (PDs).

BSFs have been proposed theoretically to act as zinc-blende quantum wells in wurtzite GaN [1], and their luminescence has been observed [2]. A built-in electric field across the BSF region has been calculated [3] and is supported by recent studies on THz radiation from non-polar GaN with high BSF density [4]. Relevant studies of stacking faults in other wurtzite materials, such as SiC, have also shown evidence of built-in electric fields [5]. However, the nature and scale of the internal electric field has not been directly determined. Here we carried out studies using high-resolution electron microscopy and electron holography to determine the microstructure of the BSFs in non-polar GaN and in particular to detect the electrostatic potential distribution across the BSF regions.

2. Experimental
The non-polar (11-20) GaN sample was grown by metal-organic vapour phase epitaxy (MOVPE) on (1-102) r-plane sapphire using trimethyl gallium (TMG), silane and ammonia (NH3) as precursors with hydrogen as the carrier gas. A more detailed description of the growth is given elsewhere [6].
The plan-view TEM specimens were prepared by mechanical polishing and Ar$^+$ ion milling. The ion milling voltage was lowered from 5 kV to 2 kV for the last 10 minutes to minimize surface damage. TEM imaging was carried out on a Philips CM30 at 200 kV and a JEOL 4000EX-II at 400 kV. A FEI Tecnai F20/Cs-corrected TEM with a Möllenstedt biprism was used to acquire high-resolution holograms at 200 kV. The fringe contrast of the reference hologram was 21-24% with a carrier frequency of 14.5 nm$^{-1}$.

3. Results and discussion

3.1. Microstructure study

The plan-view specimens of the non-polar (11-20) GaN layer were examined using bright field imaging with the $g$ vector [1-100] to show the BSFs in strong contrast (figure 1). BSFs are either terminated by PDs, or jump to an adjacent plane through the generation of PSFs. The average BSF density in this region is of the order of magnitude of 0.1 nm$^{-1}$, which is later shown to be appropriate for high-resolution electron holography study.

![Figure 1](image1.png) **Figure 1.** Bright field TEM image showing BSFs bounded by PDs and PSFs

![Figure 2](image2.png) **Figure 2.** High-resolution TEM image showing the structure of the BSFs in the non-polar GaN

High-resolution [11-20] plan-view TEM studies show the structure of the BSFs (figure 2). Although it is not straightforward to confirm the true positions of the atom columns simply from the image, the stacking sequence of the close packed planes is shown to be ...ABABACACA..., corresponding to the so-called I$_1$ type stacking fault with the displacement vector $R=1/6$ [20-23]. This has the lowest energy among all types of stacking faults in the wurtzite structure. Over 40 BSFs have been examined with high-resolution imaging on different TEM samples of this material, all of which were found to be I$_1$ type.

3.2. Electron holography investigation

High-resolution electron holography with a fringe spacing under 0.7 Å provides the spatial resolution of ~2 Å in the reconstructed amplitude and phase image, sufficient to resolve the phase distribution to atomic level. Figure 3a is a high-resolution electron hologram along the [11-20] zone axis. It shows two BSFs (indicated in regions b and c, respectively) with the stacking sequence changing from BA to AC (figure 3b), and then to CB (figure 3c). The spacing between the two BSFs is 4 nm, and no other BSFs were observed in the adjacent areas of 10 nm.
Figure 3.
(a) High-resolution electron hologram taken along the [11-20] zone axis showing two BSFs; the areas in the squares are shown magnified in:
(b) Stacking sequence changes from BA to AC
(c) Stacking sequence changes from AC to CB

The reconstruction of the hologram is shown in figure 4a and b. The phase image has been linearly tilted -0.16 rad/nm and 0.38 rad/nm in the x and y directions respectively to compensate the phase variation generated by the uniform thickness increase away from the edge. Both the amplitude and phase images show uniform and well-defined lattice planes of the specimen. Figure 4c shows the line profile perpendicular to the BSFs of the phase image. The periodic sharp peaks correspond to shielded nuclei, while the background shows the average distribution of bonding electrons as well as free carriers. Fluctuations in the background are observed at the two fault areas, which indicate that locally there may be free carrier segregation. It is possible that in the 4 nm narrow region between the two BSFs free carriers cannot fully screen the spontaneous polarization and thus the background still shows fluctuations, while in the region further away from them, the spontaneous polarization is fully screened, which leads to a flat background in the phase profile. These provide evidence for the presence of built-in electric fields across the BSF regions.

Figure 4.
(a) Amplitude and
(b) Phase image reconstructed from the electron hologram shown in figure 3a
(c) Integrated line profile of the quoted area in b. The BSFs are highlighted in all three figures.

There are, however, many uncertainties in this speculative interpretation. Contrast given by diffraction is always a concern and has not been properly removed here. Apart from this effect, however, given the spontaneous polarization of the wurtzite structure, a pair of charge "sheets" are expected at the faces of a BSF to show some phase contrast. Moreover, the peaks of the background fluctuation at the top faces of the BSFs indicate hole segregation, and therefore "valleys" in the background are expected at the bottom faces. However, these features have not been observed in our
results. On the other hand, such an experiment aiming at measurement of phase with a precision of 0.1 rad is highly sensitive to the quality of the specimen. Any artifact on or inside the sample, local thickness variation as well as charging effects under the electron beam could significantly affect the results. More experiments are necessary in this respect.

The origin of the internal electric field across a BSF is normally referred to as the result of cubic layers terminating the wurzite structure. However, there must be a change in the inter-planar spacings along the c-axis from the fault layers to the bulk material, otherwise there would simply be no internal electric field. We plan to fit the atomic positions in the high-resolution TEM image to determine the change in c-plane spacings across the BSFs, which may be as large as 5 to 10 pm [7].

4. Summary and outlook
We have studied basal-plane stacking faults in a-plane (11-20) epitaxial lateral overgrown GaN using high-resolution electron microscopy and electron holography. The structures of over 40 BSFs have been observed, all determined to be I1 type. High-resolution amplitude and phase images were obtained using off-axis electron holography. Phase fluctuations were detected at the stacking fault areas, indicating the presence of built-in electric fields. No quantitative results have been derived, however, due to uncertainties in the interpretation of the phase images.

Electron wave simulations under various tilt and defocus conditions in order to subtract the diffraction contrast are planned. DFT simulations could provide more detail about the potential distribution. For both of the simulations, precise c-plane spacing values are required, which could be obtained from atomic position fitting of the HR-TEM images.

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