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Formation of I$_2$-type basal-plane stacking faults in In$_{0.25}$Ga$_{0.75}$N multiple quantum wells grown on a (1011) semipolar GaN template

Yueliang Li, Haoyuan Qi, Tobias Meisch, Matthias Hocker, Klaus Thonke, Ferdinand Scholz, and Ute Kaiser
1Central Facility of Electron Microscopy, Electron Microscopy Group of Materials Science, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany
2Institute of Optoelectronics, Ulm University, Albert-Einstein-Allee 45, 89081 Ulm, Germany
3Institute of Quantum Matter, Ulm University, Albert-Einstein-Allee 45, 89081 Ulm, Germany

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In this work, I$_2$-type basal-plane stacking faults (BSFs) were observed in In$_{0.25}$Ga$_{0.75}$N multiple quantum wells (MQWs) grown on a (1011) semipolar GaN template by high-resolution transmission electron microscopy. The structure and formation mechanisms of the I$_2$-type BSFs at the GaN-InGaN interface were investigated in detail. The formation of the I$_2$-type BSFs contributes to lattice mismatch accommodation within the InGaN QWs. Their density varies in different regions of the sample due to the inhomogeneous distribution of the In content in the InGaN layer. The relationship between the In content in the In$_x$Ga$_{1-x}$N layer and the I$_2$-type BSFs is discussed. Published by AIP Publishing. [http://dx.doi.org/10.1063/1.4974050]

InGaN/GaN heterostructures grown on semipolar GaN templates have received considerable attention over the past years for the fabrication of light-emitting diodes (LEDs) operating in the green spectral range. For semipolar InGaN-based LEDs, the quantum confined Stark effect (QCSE), which causes the local separation of the electrons and holes in the InGaN quantum wells (QWs), can be significantly suppressed through the reduction of the polarization-related electric fields. As compared to green LEDs fabricated on conventional c-plane GaN templates, the reduced QCSE is expected to result in higher radiative recombination rate and improved overall efficiency. However, the quantum efficiency of the semipolar InGaN-based LEDs is still substantially lower than that of their blue counterparts due to the following reasons. First, the epitaxial growth of semipolar GaN templates on foreign substrates, e.g., sapphire, Si, and SiC, often yields inferior crystalline quality as compared to the conventional c-plane growth. Extended defects, i.e., threading dislocations (TDs) and basal-plane stacking faults (BSFs), formed in the semipolar GaN template, typically propagate towards the epitaxial surface and penetrate through the InGaN QWs. Second, even though the underlying GaN template is defect-free, BSFs are still possible to form in the QWs. The BSFs in the InGaN QWs, no matter whether they originated from the GaN template or at the GaN-InGaN heterointerface, give rise to fingerprint peaks in the luminescence spectra therefore deteriorating the optoelectronic properties of the InGaN-based LEDs.

Although the optimization of the GaN templates has been intensively studied, only a few reports can be found on the characterization of BSFs formed at semipolar or non-polar GaN-InGaN interfaces. Particularly, only I$_1$-type BSFs have been previously reported. However, a detailed investigation on I$_2$-type BSFs formed in semipolar InGaN QWs is still missing. In addition, the factors favoring the formation of I$_1$- or I$_2$-type BSFs remain elusive.

In this paper, we have investigated In$_{0.25}$Ga$_{0.75}$N multiple QWs (MQWs) grown on a (1011) semipolar GaN template by aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM). Despite the higher formation energy of I$_2$-type BSFs as compared to that of I$_1$-type, I$_2$-type BSFs were generally observed. The I$_2$-type BSFs originated exclusively at the GaN-InGaN heterointerfaces whereas the underlying GaN template is defect-poor. By elucidating the formation mechanism of I$_2$-type BSFs with atomic resolution, we show that the generation of I$_2$-type BSFs effectively facilitates strain relaxation within the InGaN QWs. The possible relationship between the In content in the In$_x$Ga$_{1-x}$N layer and the density as well as the type of the BSFs is further discussed.

A (1123)-oriented sapphire substrate was patterned in the following way: first, a layer of negative photoresist (approximately 1.7 μm) was spin-coated onto the surface of the sapphire substrate. Then, the photoresist was patterned by photolithography using a stripe shadow mask with an opening of 3 μm and a period of 6 μm. The stripes were oriented parallel to the in-plane m-direction of the sapphire substrate. Subsequently, trenches with 0.7 μm depth were formed by reactive ion etching (RIE) using Ar, BCl$_3$, and Cl$_2$ gases. In the next step, O$_2$ plasma cleaning was applied to remove the remaining photoresist. Finally, wet-chemical etching with KOH and piranha solution (H$_2$SO$_4$:H$_2$O$_2$) was carried out to clean the sapphire substrate. In order to avoid parasitic growth on non-c-plane-like facets, SiO$_2$ was sputtered by the shadow evaporation technique onto all the surfaces, except for one of the two (001) sidewalls.

The metal-organic vapor phase epitaxy (MOVPE) growth was conducted in a commercial Aixtron-200/4 RF-SHT reactor using the standard precursors ammonia (NH$_3$), trimethylgallium (TMGa), trimethylaluminum (TMAI), trimethylindium (TMIIn), and triethylgallium (TEGaN). On top of the (1011) GaN template, five InGaN/GaN multiple quantum well (MQW) structures were grown with a TMIIn flow rate of 64 μmol/min for the InGaN MQW growth. The growth temperatures of the MQW and barrier layers were 725 °C and 760 °C, respectively.
respectively. The QW/barrier widths were approximately 2 nm/5 nm.

For TEM investigations, cross-sectional specimens were prepared using standard techniques. The specimens were ground to a thickness of 100 μm and subsequently dimpled from both sides to less than 5 μm. Ion milling was conducted in a Fischione Ion Mill 1010 with a milling voltage of 5 kV and an inclination angle of 10°. Throughout the ion milling process, the sample stage was cooled by liquid nitrogen to reduce ion-bombardment-induced amorphization. High-resolution imaging was performed using an image-side C₄-corrected FEI Titan 80–300 microscope operated at an accelerating voltage of 300 kV. The HRTEM images were acquired under negative C₄ imaging conditions, i.e., C₄ = −13 μm and an overfocus of 6 nm.¹⁶,¹⁷

Fig. 1(a) shows an experimental [1210] overview of the TEM image of InGaN/GaN MQWs. Due to the higher atomic number of In, the InGaN layers appear darker than the GaN ones. Several extended defects can be clearly observed. As marked by the white arrows, the extended defects originate exclusively at the GaN-InGaN heterointerfaces whereas none is formed at the InGaN-GaN interfaces. Note that the extended defects exist in spite of the fact that the underlying GaN template is defect-poor. Fig. 1(b) presents the [1210] HRTEM image of one of the extended defects. Under negative C₄ imaging conditions, bright atomic columns are clearly resolved, and the stacking sequence along the c-direction could be unambiguously determined as ...ABABCACA... Here, we briefly review the three types of BSFs that exist in the wurtzite nitrides, which violate the perfect ...ABABABAB... stacking sequence along the [0001] direction. I₁-type BSF is formed by removal of a basal plane followed by ½(l110) slip of one part of the crystal (b = ½(2203)), resulting in an ...ABABCBCB... sequence. I₂-type BSF is formed either by dissociation of a perfect dislocation (b = ½(1100)) into two Shockley partials with b = ½(1100) or by ½(l110) slip of one part of the crystal with respect to another, leading to an ...ABABCACA... sequence. In I₃-type BSF, one of the A layers occupies the C position, e.g., ...ABACAB...¹³ E-type extrinsic BSF having an ...ABABCABAB... sequence is produced by insertion of an extra basal plane (b = ½[0001]).¹⁸ According to the observed stacking sequence in Fig. 1(b), the extended defect is identified as I₂-type BSF.

Fig. 2(a) shows an experimental HRTEM image near the origin of an I₂-type BSF. In order to better visualize the formation mechanism of the I₂-type BSF, Fourier filtering has been performed. Fig. 2(b) shows the Fourier-filtered image of Fig. 2(a) using 1010 and 1010 spots in the diffractogram. The fringes are broken and shifted, suggesting that the upper-left part of the crystal has slipped along the [1010] direction with respect to the upper-right part. Fig. 2(c) presents another Fourier-filtered image of Fig. 2(a) using 0002 and 0002 spots. The fringes are continuous, indicating the absence of misfit dislocation and therefore pseudomorphic growth. Based on

![FIG. 1. (a) [1210] cross-sectional overview TEM image of the InGaN/GaN MQWs showing several extended defects. (b) [1210] HRTEM image of an I₂-type BSF with the stacking sequence of ...ABABCACA... along the c-direction.](image1)

![FIG. 2. (a) An HRTEM image near the origin of an I₂-type BSF. (b) Fourier-filtered image of (a) using 1010 and 1010 spots. (c) Fourier-filtered image of (a) using 0002 and 0002 spots. (d) A model of the formation of an I₂-type BSF at the GaN-InGaN interface. The N atoms have been neglected for simplicity.](image2)
the Fourier filtering analysis, it can be concluded that the I2-type BSF is generated by a pure \( \frac{1}{3}[1010] \) slip of one part of the InGaN with respect to another. The formation mechanism of an I2-type BSF at the GaN-InGaN interface is illustrated by the schematic shown in Fig. 2(d).

The driving force of the I2-type BSF formation can be attributed to the lattice mismatch accommodation at the GaN-InGaN interfaces. According to Vegard’s law, the relaxed lattice constant of InGaN is larger than that of GaN. As shown in Fig. 2(d), the lattice mismatch along the [0112] direction can be expressed as \( \Delta d = d_{\text{InGaN}} - d_{\text{GaN}} \) for one unit cell, and \( nd\Delta d \) for \( n \) unit cells, where \( d_{\text{InGaN}} \) and \( d_{\text{GaN}} \) are the lattice spacings of InGaN and GaN along [0112], respectively. When forming an I2-type BSF, one part of the InGaN (blue) is shifted with respect to another (red) by a slip vector \( s = \frac{1}{3}[1010] \). The slip vector \( s \) has a projection on [1012], i.e., \( \frac{1}{3}j_{1012} \), which effectively reduces the average lattice spacing of InGaN in the semipolar (1011) plane. Therefore, the lattice mismatch at the GaN-InGaN interface can be partially compensated through the formation of I2-type BSFs.

As shown in Fig. 1(a), the measured distance between neighboring I2-type BSFs is approximately 10–20 nm. Distances between 50 and 100 nm were also found in other regions of the specimen (see supplementary material for more experimental images). As discussed above, the formation of I2-type BSFs is closely related to the lattice mismatch accommodation at the GaN-InGaN interfaces. Moreover, the relaxed lattice constants of In\(_x\)Ga\(_{1-x}\)N are linearly dependent on the In content \(^{19,20}\). Therefore, the density of I2-type BSFs should be dependent on the In content as well, and the correlation between them can be derived by geometrical considerations. Ideally, if \( \frac{1}{3}j_{1012} \) exactly compensates the lattice mismatch over \( n \) unit cells, the average distance between every two BSFs \( d \) is

\[
d = nd_{\text{InGaN}} - |\frac{1}{3}j_{1012}| = nd_{\text{GaN}},
\]

where \( d_{\text{InGaN}} \) and \( d_{\text{GaN}} \) are the lattice spacings of InGaN and GaN along [0112], respectively. Rewriting Equation (1) yields

\[
n = \frac{d + |\frac{1}{3}j_{1012}|}{d_{\text{InGaN}}} = \frac{d}{d_{\text{GaN}}}. \tag{2}
\]

The distance between two BSFs \( d \) is thus given by

\[
d = \frac{d_{\text{GaN}}|\frac{1}{3}j_{1012}|}{d_{\text{InGaN}} - d_{\text{GaN}}}. \tag{3}
\]

The lattice constants of GaN are \( a = 0.3189 \) nm and \( c = 0.5185 \) nm, and those of InN are \( a = 0.3548 \) nm and \( c = 0.5760 \) nm. According to Vegard’s law, the relaxed lattice constant of In\(_x\)Ga\(_{1-x}\)N can be written as \( a = 0.3189 + 0.0359x \) nm and \( c = 0.5185 + 0.0575x \) nm. After simple geometric calculation, both \( \frac{1}{3}j_{1012} \) and \( d_{\text{InGaN}} \) can be represented as functions of \( x \), whereas \( d_{\text{GaN}} \) is constant. If we first assume that the In\(_x\)Ga\(_{1-x}\)N layer is strain-free and the lattice mismatch is solely compensated by the formation of I2-type BSFs, the distance between two BSFs \( d \) can be derived by inserting the relaxed values of \( \frac{1}{3}j_{1012} \) and \( d_{\text{InGaN}} \) in Equation (3), yielding

\[
d = \frac{0.5185(0.3189 + 0.0359x) \cos 62°}{0.0575\sqrt{3}x} \text{ (nm)}. \tag{4}
\]

The solid curve in Fig. 3 shows the correlation between \( d \) and \( x \) calculated by using Equation (4). Since the lattice mismatch increases with the increase in In content, a higher density of BSFs is required for lattice mismatch accommodation, leading to a reduced distance \( d \). It is worth noting that the InGaN layer is compressively strained to the GaN layer (Fig. 2(c)), resulting in a reduction of \( d_{\text{InGaN}} \) and \( |\frac{1}{3}j_{1012}| \) in Equation (3). Therefore, in order to take the compressive strain into consideration, we have incorporated strain-correction in the calculation by reducing the values of \( d_{\text{InGaN}} \) and \( |\frac{1}{3}j_{1012}| \). The dotted curves in Fig. 3 present the calculated \( d-x \) correlations when the In\(_{0.25}\)Ga\(_{0.75}\)N sample is under 1%, 2%, and 3% compressive strain. The curves are right-shifted showing lower BSF density in the strained In\(_{0.25}\)Ga\(_{0.75}\)N layer. Nevertheless, the dependence of BSF density on the In content is similar in both relaxed and strained cases. Based on the experimental HRTEM images, the average distance between two I2-type BSFs in our In\(_{0.25}\)Ga\(_{0.75}\)N sample is determined to be approximately 35 nm. The experimental data point is marked in Fig. 3.

The formation of I1-type BSFs has been reported in In\(_{0.25}\)Ga\(_{0.75}\)N/GaN MQWs grown on the (1011) semipolar GaN template.\(^6\) However, in our sample, only I2-type BSFs were observed. An I1-type BSF is formed by the removal of a basal plane generating an edge dislocation with the Burgers vector of \( b = \frac{1}{4}[0001] \), followed by a \( \frac{1}{2}[1100] \) slip. Both the Burgers vector and the slip vector have projections on the (1011) plane, therefore contributing to the lattice mismatch accommodation. The compensation of an I1-type BSF can then be represented as \( \frac{1}{6}a \cos 62° + \frac{1}{2}c \sin 62° \), where \( a \) and \( c \) are the lattice constants of In\(_x\)Ga\(_{1-x}\)N, and 62° is the angle between (0001) and (1011) planes. For an I2-type BSF, the compensation can be expressed as \( |\frac{1}{3}j_{1012}| = \frac{1}{\sqrt{3}}a \cos 62° \). It is clear that the lattice mismatch compensation induced by I1-type BSF is higher than that of I2-type BSF. However,
since the elastic energy of a dislocation is proportional to \( b^2 \), the local strain energy of an I\(_1\)-type BSF is also higher than that of an I\(_2\)-type BSF. The comparison of \( b^2 \) and compensation between the two types of BSF are shown in Table I. As a result, the type of BSF formed at the GaN-InGaN interface depends on both the magnitude of lattice mismatch and the extra elastic strain energy introduced by InGaN interface.

<table>
<thead>
<tr>
<th>BSF type</th>
<th>Burgers vector ( b )</th>
<th>( b^2 )</th>
<th>Compensation</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(_1)</td>
<td>( \frac{1}{3}(1010) )</td>
<td>( \frac{2}{9} )</td>
<td>( \frac{a}{\sqrt{3}} \cos62^\circ )</td>
</tr>
<tr>
<td>I(_2)</td>
<td>( \frac{1}{2} + \frac{1}{3}(1010) )</td>
<td>( \frac{2}{9} + \frac{2}{9} )</td>
<td>( \frac{1}{2}\sin62^\circ + \frac{a}{2\sqrt{3}} \cos62^\circ )</td>
</tr>
</tbody>
</table>

Table I. Comparison of the crystal movement and compensation between the two types of BSF.

We gratefully acknowledge financial support from the DFG (KA1295-19) and technical support from Sabine Grözinger in cross-section TEM sample preparation.

See supplementary material for more experimental images of I\(_2\)-type BSFs with various densities.

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