Single crystalline Sc$_2$O$_3$/Y$_2$O$_3$ heterostructures as novel engineered buffer approach for GaN integration on Si (111)

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The preparation of GaN virtual substrates on Si wafers via buffer layers is intensively pursued for high power/high frequency electronics as well as optoelectronics applications. Here, GaN is integrated on the Si platform by a novel engineered bilayer oxide buffer, namely, Sc$_2$O$_3$/Y$_2$O$_3$, which gradually reduces the lattice misfit of $\sim-17\%$ between GaN and Si. Single crystalline GaN(0001)/Sc$_2$O$_3$(111)/Y$_2$O$_3$(111)/Si(111) heterostructures were prepared by molecular beam epitaxy and characterized ex situ by various techniques. Laboratory-based x-ray diffraction shows that the epitaxial Sc$_2$O$_3$ grows fully relaxed on the Y$_2$O$_3$/Si(111) support, creating a high quality template for subsequent GaN overgrowth. The high structural quality of the Sc$_2$O$_3$ film is demonstrated by the fact that the concentration of extended planar defects in the preferred (111) slip planes is below the detection limit of synchrotron based diffuse x-ray scattering studies. Transmission electron microscopy (TEM) analysis reveal that the full relaxation of the $-7\%$ lattice misfit between the isomorphic oxides is achieved by a network of misfit dislocations at the Sc$_2$O$_3$/Y$_2$O$_3$ interface. X-ray reflectivity and TEM prove that closed epitaxial GaN layers as thin as 30 nm can be grown on these templates. Finally, the GaN thin film quality is studied using a detailed Williamson–Hall analysis. © 2010 American Institute of Physics. [doi:10.1063/1.3485830]

I. INTRODUCTION

Integration of GaN on the Si platform has high potential to improve the performance of Si circuits by adding new functionalities, enabling better high power and high frequency electronics [e.g., GaN high electron mobility transistor with Si complementary metal-oxide semiconductor (CMOS)] as well as opening new opportunities in the fields of optoelectronics (e.g., GaN-based laser with Si CMOS).$^{1-4}$ The use of large-size Si wafers as substrates for GaN creates furthermore a cost advantage with respect to currently used methods of GaN epitaxy on small-size, expensive SiC, and sapphire substrates. The challenge is to develop a manufactur- process for crack free, low dislocation density GaN films on large diameter Si wafers. Currently, two main approaches aiming at this target are layer transfer$^{5,6}$ and heteroepitaxial thin film deposition techniques.$^7$ However, the layer transfer method (e.g., Smart Cut™) suffers from the fact that no single crystal GaN can be grown at a reasonable price, to provide a source for high quality GaN thin films. In this respect, it is at present the heteroepitaxy approach which results in an economic relationship between cost and quality. Nevertheless, it is extremely difficult to grow GaN directly on Si substrates due to the large lattice mismatch ($\sim-17\%$) and the difference in thermal expansion coefficients ($\sim-55\%)$. In addition, Si is well known to heavily react with impinging Ga. To accommodate the misfit and avoid interfacial reactions, different semiconducting buffer layers including AlN,$^{9,10}$ AlN/GaN multilayers$^9$ as well as AlGaN$^{12,13}$ were used in the past.

Recently, the rich physics and chemistry of oxide heterostructures was exploited to grow a flexible buffer system for Si and Ge integration on Si wafers.$^{14,15}$ Indeed, the use of oxide buffers could also be beneficial for GaN integration on Si (Ref. 16) (e.g., substrate loss reduction in case of high frequency applications) and a number of oxides such as ZnO,$^{17,18}$ $\gamma$-Al$_2$O$_3,$$^{19,20}$ and Sc$_2$O$_3$ (Ref. 21) were recently tested. However, the limited stability of ZnO with respect to the N-source turned out to be problematic for high quality GaN growth at elevated temperatures.$^{22}$ Furthermore, $\gamma$-Al$_2$O$_3$(111) grown on Si(111) exhibits two types of stacking domains, which can lead to the formation of defects in GaN film.$^{23}$ First promising results concerning GaN epitaxy on Sc$_2$O$_3$/Si(111) supports were reported.$^{24,25}$ The advantage of this approach is a high stability of the GaN/Sc$_2$O$_3$ interface. However, the large lattice mismatch between Sc$_2$O$_3$ and Si can result in a high defect density in the Sc$_2$O$_3$ buffer and might limit the GaN layer quality.

In this work, we investigate the growth of GaN on Si(111) using a novel engineered bi-layer buffer composed of two different bixbyite oxides (space group $Ia\overline{3}$), namely, Y$_2$O$_3$ and Sc$_2$O$_3$.

According to the bulk crystal lattices, since Y$_2$O$_3$ has an in-plane lattice misfit of $-2\%$ to Si, Sc$_2$O$_3$ $-7\%$ to Y$_2$O$_3$ and GaN $-8\%$ to Sc$_2$O$_3$, the lattice misfit between GaN and the substrate can be theoretically reduced from $17\%$
(GaN/Si) to 8% (GaN/Sc₂O₃). The idea is to grow fully relaxed Sc₂O₃ films of high structural quality on Y₂O₃/Si(111) supports for subsequent GaN overgrowth. This requires that the lattice misfit of about 7% between the isomorphic oxides is released by a vernier lattice of misfit dislocations (MD), running preferentially in the Sc₂O₃/Y₂O₃ interface. Additionally, the Sc₂O₃/Y₂O₃ buffer needs to fulfill a number of further requirements: (a) ensure electrical isolation, (b) assure high temperature stability for GaN overgrowth, and (c) suppress GaN/Si interface reactions.

As main result, it is found in the present paper by complex laboratory and synchrotron x-ray diffraction (XRD) analyses that the growth of truly single crystalline GaN/Sc₂O₃/Y₂O₃/Si(111) heterostructures is feasible. The novel buffer approach is proven to result in fully relaxed Sc₂O₃ films on Y₂O₃/Si(111) supports with structural defect concentrations of preferred orientation (e.g., stacking faults on {111} slip planes) in the oxide films below the detection limit of modern 3rd generation synchrotron sources. Furthermore, the single crystalline GaN films are closed at a film thickness as low as 30 nm and can be grown at elevated temperatures on the engineered oxide buffer on Si(111).

II. EXPERIMENTAL

The 4-in. boron-doped Si (111) wafers were used as substrates. To obtain atomically smooth Si surfaces, the wafers were cleaned by the standard piranha procedure and etched in NH₄F according to a previously described recipe. Prior to the deposition, substrates were annealed in ultrahigh vacuum (UHV) for 5 min at 700 °C to obtain high quality (7 × 7)-Si(111) surfaces.

GaN/Sc₂O₃/Y₂O₃/Si(111) heterostructures were prepared in a multicrystal molecular beam epitaxy (MBE) system without breaking the vacuum. Substrate temperature during growth of Y₂O₃ and Sc₂O₃ was 650 °C and 500 °C, respectively. The respective average growth rates were 1.5 nm/min and 2.5 nm/min. Pressure in the oxide chamber during deposition was in the order of 10⁻⁶ mbar. After oxide deposition, samples were transferred under UHV to another MBE chamber for plasma assisted GaN growth. During GaN deposition, substrate temperature, growth rate, and III–V chamber pressure were 650 °C, 1 nm/min, and 10⁻⁵ mbar, respectively. During the growth, nitrogen was supplied through a radio frequency plasma source operated at an input power of 250 W.

A Philips CM300 transmission electron microscope (TEM) operated at 300 kV with a resolution of 0.2 nm was used as a local probe to measure direct cross-sectional lattice images of the heterostructures. TEM photographs were taken along the bulk Si(111) direction. To obtain global information about the sample structure, laboratory based x-ray reflectivity (XRR) and XRD studies were carried out using a Rigaku Smartlab diffractometer with Cu Ka radiation (λ = 1.542 Å).

To gain further insight into the structural features of the heterostructures, synchrotron-based XRD studies were performed at the insertion device 32 beamline of the European synchrotron radiation facility in Grenoble (France). Here, a Kappa-Six circle diffractometer was used in the grazing incidence (GI) mode with an x-ray beam energy of 15 keV (λ = 0.8265 Å). For the used wavelength, the critical angles of incidence for Si, Y₂O₃, Sc₂O₃, and GaN are 0.119°, 0.163°, 0.15°, and 0.18°, respectively. This results in bulk sensitive measurements at an incident angle αi = 0.2°, and surface sensitive studies at αi = 0.1°. For αi = 0.1°, the theoretical penetration depth in the GaN was calculated to be about 2.5 nm. For GI-XRD the hexagonal Si(111) surface coordinate system in reciprocal space is used with H, K, L pointing in the directions [2110], [2111], and [111] of the bulk Si lattice, respectively.

III. RESULTS AND DISCUSSION

Figure 1 shows XRR and XRD scans performed in the specular θ-2θ geometry on GaN/Sc₂O₃/Y₂O₃/Si(111) heterostructure. XRR oscillations [Fig. 1(a)] for the selected sample can be very well fitted using a three layer GaN/Sc₂O₃/Y₂O₃ model without any transition regions. This result especially indicates that the GaN film is closed and of only limited roughness. Extracted layer thicknesses and relative electron densities are indicated in the inset to Fig. 1(a) (dashed lines denote Y₂O₃, Sc₂O₃, and GaN bulk densities). In case of the measured sample, the extracted Y₂O₃, Sc₂O₃, and GaN layer thicknesses are 5 nm, 25 nm, and 30 nm, respectively. The GaN surface roughness is about 1.5 nm.

To determine the growth orientation of the heterostack, a specular θ-2θ XRD scan over an angular 2θ range from 20° to 130° was performed [Fig. 1(b)]. Peak positions are indicated by the dashed lines. (111) diffraction peaks of different order n are clearly seen for the Si substrate (n = 1, 2, 3) and for the Y₂O₃ and Sc₂O₃ layers (n = 2, 4, 6). Bragg peaks of the hexagonal phase of GaN. The deduced vertical growth orientation is in consequence as follows: GaN(0001)/Sc₂O₃(111)/Y₂O₃(111)/Si(111). The unit cell
parameters calculated from the Y$_2$O$_3$ (444) and Sc$_2$O$_3$ (444) peak positions agree with fully relaxed cubic lattices and are 10.635 Å and 9.846 Å, respectively. The GaN lattice parameter $c$ extracted from the GaN(0004) reflection is 5.176 Å. Thus, the experimental lattice constant of GaN is slightly smaller than the theoretical value (5.186 Å). This behavior is possibly caused by an in-plane tensile strain in the GaN film, as discussed in more detail below.

The azimuthal orientation of the GaN(0001)/Sc$_2$O$_3$(111)/Y$_2$O$_3$(111)/Si(111) heterostructure was studied by Synchrotron radiation-GIXRD in-plane measurements performed at L=0.03 r.l.u. (reciprocal lattice unit). The incident angle $\alpha_i$ of the x-ray beam was varied from 0.2° (bulk sensitive) to 0.1° (surface sensitive). Figure 2 shows the scans along the K-axis (corresponding to Si[211]) with K ranging from 0.5 to 6.2 r.l.u. The top curve, obtained with an incident angle of 0.2°, gives information about the entire heterostructure. The allowed Si(422) and Si(844) Bragg peaks from Si(111) substrate are expected at K=3 r.l.u. and K=6 r.l.u., respectively. Due to the fact that the Y$_2$O$_3$ layer is 5 nm thin, only one weak Y$_2$O$_3$(844) reflection is detected at K=3.081 r.l.u. The weak and rather broad signal does not allow a further precise discussion of the in-plane Y$_2$O$_3$ lattice parameter constant. In addition, five Sc$_2$O$_3$ reflections are detected at K=0.83, 1.66, 2.49, 3.32, and 4.98 r.l.u. These peaks are attributed to Sc$_2$O$_3$(221), (422), (633), (844), and (1266) Bragg peaks, respectively. The lattice constant calculated from the high order Sc$_2$O$_3$(844) peak position agrees with the fully relaxed cubic lattice and is 9.50 Å. Diffraction signals of the GaN layer are found at K=1.19, 2.38, 3.57, and 4.76 r.l.u. and are attributed to the GaN(1010), (2020), (3030), and (4040) Bragg peaks, respectively. Furthermore, the bulk sensitive scan nicely demonstrates the role of the oxide buffer as lattice mismatch mediator: its Y$_2$O$_3$(844) and Sc$_2$O$_3$(844) Bragg peaks are situated between Si(422) and GaN(3030) diffraction signals. The following conclusions can be drawn:

- As seen by the Y$_2$O$_3$(844) and Sc$_2$O$_3$(844) Bragg peaks, the oxide films match each other on the basis of a (1×1) coincidence but the Sc$_2$O$_3$ lattice is by about 7% smaller.
- In addition, it can be deduced from the Sc$_2$O$_3$(844) and GaN(3030) peak positions that 1/3 $d$$_{\text{GaN}}$$^{1010}$ is by about 8% smaller than 1/4 $d$$_{\text{Sc}_2\text{O}_3}$$^{111}$. This rather complicated epitaxial relationship is currently investigated by theoretical ab inito studies (adsorption sites, etc.).

A second in-plane scan was performed along the K direction in the surface sensitive mode at $\alpha_i$=0.1° (Fig. 2). Based on the fact that the diffraction signals from Si and buffer oxides are fully suppressed and only four GaN reflections are visible, it is clearly demonstrated that the epitaxial GaN forms a closed layer on a global scale. From the position of the GaN Bragg peaks, it can be stated that the 30 nm thick GaN film exhibits a tensile strain of the hexagonal GaN unit cell by about 0.6% ($a_{\text{GaN bulk}}=3.18$ Å, $a_{\text{GaN layer}}=3.20$ Å). The in-plane tensile stress is probably exerted by the bigger oxide buffer/Si heterostructure underneath.

The out-of plane Phi ($\phi$) scans, shown in Fig. 3, were carried out across Si[111], Y$_2$O$_3$(222), Sc$_2$O$_3$(222), and GaN[1011] reflections to determine the stacking configuration of the heterostructure. These measurements were accomplished by fixing the diffraction angle 2$\theta$ and the inclination angle $\chi$ to the desired reflection and performing in-plane 360° $\phi$ scans around the Si[111] surface normal. The three-fold off-plane symmetry of the Si(111) and cubic (111) oxide films is evident from the observed 120° spacing between Si and oxides reflections, respectively. Furthermore, the 60° off-set between Si(111), Y$_2$O$_3$(222), and Sc$_2$O$_3$(222) Bragg peaks indicate that the oxides grow epitaxially on Si(111) with a type-B orientation. Here, let us recall that type-A denotes a (111)-oriented fcc-like epilayer, whose (111) planes exhibit the same stacking vector as the Si(111) substrate. On the contrary, type-B refers to the case in which a stacking fault at the epilayer/Si(111) interface rotates the stacking vector in the growing film by 180° around the Si(111) surface normal. The detected 60° spacing between GaN[1011] reflections confirms the hexagonal symmetry of the GaN unit cell. Summarizing the results of Figs. 2 and 3, the epitaxial in-plane alignment of the heterostruc-
nature is characterized by the relationship: GaN[1010]|Sc2O3[211]|Y2O3[211]|Si[211].

Figure 4 shows a reciprocal space map (RSM) for the GaN(0001)/Sc2O3(111)/Y2O3(111)/Si(111) heterostructure in the H-L plane. The sketch in the top part of this figure represents all expected reflections in the L range from 0.0 to 0.85 r.l.u. and H range from −0.75 to −2.7 r.l.u., according to the epitaxial out-of-plane and in-plane relationships derived from the studies presented in Figs. 1–3. In this H-L region of reciprocal space, a bulk sensitive mesh scan with αs=0.4° was performed. The detected Si, Y2O3, Sc2O3, and GaN peak positions are in very good agreement with those theoretically predicted. Moreover, no additional reflections, which would indicate the presence of misoriented grains (e.g., inclusion of cubic GaN) or possible mixed phases (due to, e.g., interface reactions) are observed. However, the diffuse scattering around the GaN Bragg peaks clearly indicates the presence of defects causing a tilt and twist of the GaN lattice.

Here, we restrict ourselves to the analysis of the diffuse scattering around the oxide Bragg peaks in Fig. 4 to evaluate the presence of structural defects of preferred orientation, e.g., stacking faults on {111} planes in the oxide buffer. It was shown by Zaumseil and co-workers31 that such stacking faults can be identified in the RSMs of bixbyite oxide (222) Bragg peaks (e.g., Pr2O3) by elongated streaks along {111} directions. To discuss this in more detail, an equivalent RSM for the Sc2O3/Y2O3 buffer layer system. The in-plane a∥ and out-of-plane a⊥ lattice parameters can be extracted by intercepting the linear regression of such experimental points at cos2(χ)=0 and 1, respectively. The Si, 1/2 Y2O3, and 1/2 Sc2O3 cubic bulk lattice constant values are marked with horizontal solid lines. It can be seen that the a∥ and a⊥ lattice parameters for the 6 nm thick Y2O3 layer are within the experimental error of the same value and very close to the bulk lattice constant. Similar behavior is observed for the 20 nm thick Sc2O3. This implicates that the Y2O3 and Sc2O3 films are nearly fully relaxed. The lack of strain in especially the Sc2O3 layer indicates two results. First, the fully relaxed the novel engineered Sc2O3/Y2O3 buffer approach on Si(111) provides a template of high structural quality for GaN overgrowth.

The strain state of the oxide layers can be analyzed by means of an XRD technique which identifies the presence of tetragonal distortions in heteroeptaxially grown cubic layers. This method is based on calculating a cubic unit cell lattice constants from differently tilted diffraacting netplanes.34 The angle χ is the angle between the sample surface (111) and the tilted (h k l) netplane. Assuming an undistorted cubic lattice, a hypothetical cubic unit cell constant is calculated from the d-spacing of the Bragg peaks of the various tilted lattice planes. These values are plotted as a function of cos2(χ). For example, the out-of-plane Bragg planes (χ=0°) are plotted at cos2(χ)=1, the in-plane Bragg planes (χ=90°) are plotted at cos2(χ)=0. Figure 6 shows the results of such an analysis for the Sc2O3/Y2O3 buffer layer system. The in-plane a∥ and out-of-plane a⊥ lattice parameters can be extracted by intercepting the linear regression of such experimental points at cos2(χ)=0 and 1, respectively. The Si, 1/2 Y2O3, and 1/2 Sc2O3 cubic bulk lattice constant values are marked with horizontal solid lines. It can be seen that the a∥ and a⊥ lattice parameters for the 6 nm thick Y2O3 layer are within the experimental error of the same value and very close to the bulk lattice constant. Similar behavior is observed for the 20 nm thick Sc2O3. This implicates that the Y2O3 and Sc2O3 films are nearly fully relaxed. The lack of strain in especially the Sc2O3 layer indicates two results. First, the fully relaxed
Sc$_2$O$_3$ film on Y$_2$O$_3$/Si(111) support achieves its bulk unit cell constant so that the lattice mismatch between GaN and Sc$_2$O$_3$ is reduced to the smallest possible value. Second, the theoretical lattice mismatch of $-7\%$ between the oxide layers must be relaxed by the formation of a network of MD at the oxide/oxide interface.

This is investigated in more detail by cross-sectional TEM images (in Si(110) direction) shown in Fig. 7. The TEM image shown in Fig. 7(a) confirms the closed nature of the GaN layer. The thicknesses of the layers constituting the heterostructure are well in line with the values extracted from XRR. Figure 7(b) shows a high magnification image of the interface regions between the Y$_2$O$_3$ and Sc$_2$O$_3$ as well as the Sc$_2$O$_3$ and GaN layers. At the interface between the buffer oxides, MD are clearly visible. The formation mechanism of such defects is illustrated in Fig. 7(c). To accommodate the difference in the lattice constants between Y$_2$O$_3$ and Sc$_2$O$_3$, for every 10 Y$_2$O$_3$ atomic planes 11 Sc$_2$O$_3$ atomic planes are formed in the (111) direction, with a theoretical lattice mismatch of 7% between the oxide layers.

MD at the interface between Y$_2$O$_3$ and GaN must be relaxed by the formation of a network of MD at the interface. The vernier period of dislocation $p$ is about 2.5 nm which is in agreement with theoretical calculations for a fully relaxed Sc$_2$O$_3$/Y$_2$O$_3$ heterostructure. The TEM cross section confirms also that the buffer oxides are type-B with respect to the Si substrate (as it was derived by the $\phi$ scans in Fig. 3). This can be seen from the stacking faults at the Y$_2$O$_3$/Si(111) boundary, as explained in more detail in Ref. 36. Finally, based on the TEM study it is concluded that no interface reactions are formed either between Si and Y$_2$O$_3$ or between Sc$_2$O$_3$ and GaN.

Further information regarding the quality of the heterostructure can be extracted from the RSMs shown in Figs. 8(a) and 8(b). Note that the RSM is obtained by taking a series of $\omega$ scans at successive $\omega$-2$\theta$ values and presenting the results as a map. In order to plot such a map, the angles from radial and angular scans are converted into reciprocal lattice units. Figure 8(a) shows the RSM of the out-of-plane Si(111), Y$_2$O$_3$(222), Sc$_2$O$_3$(222), and GaN(0002) reflections. The coordinates $Q_z$ and $Q_x$ can be expressed as: $Q_z =$ [sin($\omega$)+sin(2$\omega$-$\omega$)]/\lambda, $Q_x =$ [cos(2$\theta$-$\omega$)-cos($\omega$)]/\lambda (Ref. 37) and point in the Si[111] and Si[211] directions in real space, respectively. It is noted that the Y$_2$O$_3$(222) Bragg peak is too weak to be analyzed and it is not further discussed. It is seen that Sc$_2$O$_3$(222) and GaN(0002) peaks show an anisotropic shape with smaller and bigger full width at half maximum (FWHM) values and presenting deeper insights in the structural perfection of the Sc$_2$O$_3$ and GaN film, a Williamson Hall analysis was performed. For this analysis, besides the RSM in Fig. 8(a), radial and angular scans were measured for the investigation of higher order reflections. The out-of-plane results of this method are presented in Fig. 8(b). Here, the FWHM values $\Delta Q_z$ and $\Delta Q_x$ for Sc$_2$O$_3$(222), (444), (666) and GaN(0002), (0004), (0006) are plotted as a function of peak position $Q_z$ in reciprocal space and linear regressions for each of the four data sets were performed. The intercept resulting from fitting the $\Delta Q_z$ ($\Delta Q_x$) data is inversely proportional to the domain sizes $D_z$ ($D_x$) in the $Q_z$ ($Q_x$) direction, respectively. From the slope of the linear fits of $\Delta Q_z$ and $\Delta Q_x$, the average vertical strain variation and the tilt of the mosaic blocks, respectively, can be obtained. The Sc$_2$O$_3$ and GaN domain sizes calculated from the FWHM analysis of the $Q_z$ values are 27 nm and 30 nm, respectively. These values are close to the GaN and Sc$_2$O$_3$ layer thicknesses measured by XRR. A small average vertical strain variation of about 0.26% in the Sc$_2$O$_3$ and 0.28% in the GaN layer from the slope of the $\Delta Q_z$ values is detected. It is worth noting that strain variation is a manifes-
The RSM of the in-plane Si(422), Y$_2$O$_3$(844), Sc$_2$O$_3$(844), and GaN(030) reflections is shown in Fig. 8(c). Here, the $Q_x$ and $Q_y$ are defined as: $Q_x = [\sin(\omega) + \sin(2\theta - \omega)]/\lambda$, $Q_y = [\cos(2\theta - \omega) - \cos(\omega)]/\lambda$ and correspond to the Si[211] and Si[110] directions, respectively. Similarly, the RSM shown in Fig. 8(a), the Sc$_2$O$_3$(844) and GaN(030) peaks exhibit an anisotropic shape with FWHMs higher in $Q_x$ than in $Q_y$. In the present case, the broadening of the peaks in the $Q_x$ and $Q_y$ directions is found to be 42 nm and 38 nm, respectively. The corresponding values for GaN are 31 nm and 37 nm, respectively. The slope of the linear fits of $\Delta Q_x$ and $\Delta Q_y$ provides information about the average in-plane strain variation and the twist of the mosaic blocks, respectively. For the Sc$_2$O$_3$ layer, the in-plane strain variation and the twist angle amounts to 0.7% and 1.6°, respectively. For the GaN layer the in-plane strain variation is 1.3%, and the twist amounts to 2.4°. The twist angle of about 2.4° is probably a manifestation of a relatively high edge dislocation content in the GaN film. Based on the above Williamson–Hall analysis, it is concluded that the thin GaN layer is characterized by larger strain variations and higher values of lattice tilt and twist in comparison with the Sc$_2$O$_3$ buffer layer.

IV. CONCLUSIONS

In summary, a “proof of principle” study to integrate single crystalline GaN on the Si(111) platform via an engineered Y$_2$O$_3$/Sc$_2$O$_3$ buffer system was demonstrated by advanced laboratory and synchrotron-based XRD measurements. Specular θ-2θ scans reveal that the vertical growth orientation of the heterostructure is GaN(0001)/Sc$_2$O$_3$(111)/Y$_2$O$_3$(111)/Si(111). The in-plane orientation is defined by GaN[1010]∥Sc$_2$O$_3$(211)∥Y$_2$O$_3$(211)∥Si[211]. The Y$_2$O$_3$ and Sc$_2$O$_3$ buffer oxides are of type-B stacking orientation with respect to the Si(111) substrate and are fully relaxed. The 7% lattice mismatch between the oxides is compensated by edge dislocations formed by insertion of additional [111] planes in the Sc$_2$O$_3$ thin film. Diffuse x-ray scattering studies using a 3rd generation synchrotron source prove that densities of extended structural defects of prefered [111] orientation in the Sc$_2$O$_3$ layer are below the detection limit. In other words, the novel engineered Sc$_2$O$_3$/Y$_2$O$_3$ buffer approach results in fully relaxed Sc$_2$O$_3$ films of high structural quality for GaN overgrowth. Based on in-plane and out-of-plane XRD scans, it is concluded that 30 nm GaN layers grown on Sc$_2$O$_3$/Y$_2$O$_3$ buffers are under tensile strain. According to the Williamson–Hall analysis, the very thin GaN films exhibit after the island coalescence process a high content of screw and edge dislocations. Certainly, the GaN film crystal-
linity is related to the quality of the initial nucleation layer and in particularly to the nature of the atomic bonding between $\text{Sc}_2\text{O}_3$ and GaN.\textsuperscript{41,42} Therefore, \textit{in situ} growth studies by reflection high-energy electron diffraction, X-ray photoemission spectroscopy (XPS), and ultraviolet photoemission spectroscopy are under way to unveil the mostly unknown growth behavior of GaN on $\text{Sc}_2\text{O}_3$. Furthermore, the optimization of the initial GaN island coalescence process, similar to the nucleation phase of GaN on sapphire substrates,\textsuperscript{43} is important to improve in future studies the defect densities of GaN layers. These future studies, in combination with thermal mismatch engineering, are of special importance to evaluate the technological potential of the GaN integration approach via $\text{Sc}_2\text{O}_3$/Y$_2$O$_3$ buffers on Si(111) with respect to the state-of-the-art in GaN fabrication on foreign substrates (such as SiC and sapphire).