Lattice distortion induced by strain can change the bandgap of GaN, which can affect the device properties.  

For semiconductor device fabrication, an understanding of this lattice distortion has become critical as the device size becomes increasingly smaller. Among the many available methods for evaluating this lattice distortion, X-ray diffraction topography (XRDT) is of particular interest, because it has provided information regarding lattice-plane tilt angles in a diffraction plane,6–9 as well as dislocations7 since the development of the Berg–Barrett topography method.7,8 By combining XRDT with a laser scanning method, it is possible to obtain a precise surface normal direction including the residual stress.5 A recent X-ray diffraction study on the lattice plane bending of a 4H-SiC substrate provided the shape and curvature of the substrate.6 However, no information on the three-dimensional (3D) mapping of the reciprocal space vector, such as \( q_x \), \( q_y \), and \( q_z \), at each point in the wafer has been reported, owing to the measurement time and cost limitations. To date, it has been impossible to obtain such information on the lattice-plane orientation from a whole wafer using the other methods.

Obtaining lattice plane information, such as the curvature and orientation, is also important for the fabrication of light-emitting diodes (LEDs). Even though the recent invention of blue LEDs based on GaN greatly improved the quantum efficiency and feasibility of GaN,9 issues concerning the lattice mismatch still exist. In general, GaN epitaxial layers are grown on other materials such as a Si,10 SiC,11,12 and sapphire substrates.13 However, these hetero-epitaxial layers result in lattice mismatch and strain,10–13 which degrade the device performance. Recently introduced hydride vapor phase epitaxy methods allow the fabrication of GaN layers on GaN substrates, which are commercially available.14 Ideally, growing GaN layers on a GaN substrate is the optimal approach for minimizing the lattice mismatch and strain effect. Despite this progress, it remains difficult to obtain high-quality layers, which means that the lattice mismatch and strain issues have not yet been solved. For these reasons, a better understanding of the lattice-plane orientation of GaN layers on the wafer scale is needed. N-channel GaN metal–oxide–semiconductor field-effect transistors were homeopitaxially fabricated on bulk GaN substrates, and excellent characteristics were reported.15 The uniform quality of Mg-doped GaN layers on whole bulk GaN substrates is required in order to increase the yield. Therefore, wafer-scale crystal characterization of homeopitaxial p-GaN layers is critically important.

In this study, we propose the use of grazing-incidence XRDT combined with a reciprocal lattice vector \( q \) and a rotation matrix. Moreover, we provide the \( q_x \), \( q_y \), and \( q_z \) information at every point in the wafer.

The sample was a 2-µm-thick Mg-doped GaN layer with a concentration of \( 1 \times 10^{17} \, \text{cm}^{-3} \) grown on a 1-µm-thick undoped GaN layer on a 330-µm-thick GaN(0001) substrate of a 2-in.-diameter wafer. The flat notch direction was \( 2 \theta = 1100 \), and the direction perpendicular to the flat notch was \( 1120 \). To obtain a topography image in reflection mode, we used XRDT at BL20B2 SPring-8, Japan. The wavelength of the incident X-rays was 1.284 Å, selected by a Si(111) double-crystal monochromator. The incident X-ray beam was highly parallel in the vertical direction, and its calculated angular divergence was 29.8 prad. The incident beam size was adjusted to be 1.5 mm (h) × 100 mm (v), which was larger than the 2-in. wafer. A flat panel sensor (FPS) detector (Hamamatsu Photonics C7942) with a pixel size of 50 × 50 µm² and a resolution of 2368 × 2240 was used for the image acquisition. The X-ray exposure time was set to 0.5 s, which was sufficient for obtaining the diffraction signal. A dark image without incident X-rays was measured prior to the acquisition of diffraction images for the background subtraction.

Figure 1(a) presents a schematic of the grazing-incidence XRDT setup. The diffraction angle denoted as \( 2 \theta \) was adjusted to be 79.3° for the GaN 1124 reflection. Here, we assumed that the GaN substrate had a curved lattice plane with the same \( d \)-spacing. After positioning the FPS detector at the \( 2 \theta \) angle, we placed the GaN substrate at an incident angle \( \theta \) of approximately 0.6°. Under these conditions, the diffracted X-ray directly entered the FPS detector, Fig. 1(b) shows the
partially diffracted image originating from the lattice orientation inclination. To obtain the rocking curve at every point, we adjusted the incident angle by rotating the sample to ±30° with steps of 25 arcsec at the fixed detector position. The partially diffracted images were stacked to form a 3D matrix for analysis of the rocking curve at every \((x, y, \theta_z)\) point. A peak of the rocking curve is located at \(\theta_0(x, y, \phi)\). \(\phi\) is an azimuthal angle around the sample surface normal. We can introduce an average value \(\theta_{ave}(\phi)\) defined as \(\langle \Sigma_{x,y}\theta_0(x,y,\phi) \rangle\). For obtaining rocking-curve maps and in-plane \(q\) components at the same 2\(\theta\) angle, the same measurement procedure was applied to the sample at \(\phi = 120^\circ\). This is because a GaN single crystal has threefold symmetry in the [0001] direction, and its space group is \(P6_3/mmc\).

Let us write the conditions for application of the proposed method. The GaN wafer for our experiment had a high crystal quality, and the lattice constant was almost unique over the wafer. If the lattice constant has large variations and distributions, the origin of the 2\(\theta\) variations is ambiguous. In this condition, one image pixel contains information about many \(d\)-spacings. For this reason, a sample having high crystal quality is desired for our proposed method. According to the Bragg law, we use the formula \(\delta d/d = -(\cos\theta_0/\sin\theta_0)d\delta\theta\) for a monochromatic X-ray beam. By introducing \(\Delta p\) (pixel size) and \(L\) (camera distance from substrate to detector), we can rewrite the formula as \(|\delta d/d| < \Delta p/(2L \tan\theta_0)\). In our experiment, \(\Delta p, L, \text{ and } \theta_0\) were 50 \(\mu\)m, 0.5 m, and 39.67°, respectively, leading to \(|\delta d/d| < 6.0 \times 10^{-5}\). The \(d\)-spacing of GaN(1124) lattice planes is 1.006 Å; thus, \(|\delta d|\) should be smaller than 6.0 \(\times 10^{-5}\). If the \(|\delta d|\) of a sample is larger than this value, the assumption is still valid if the binning of the FPS pixel is performed. From a similar consideration of the lateral space resolution, we have a limitation regarding the angular deviation \(\Delta \psi\) of a local \(q\) vector from the average normal of a lattice plane almost parallel to the sample surface. We can observe \(|\Delta \psi| < \Delta p/L \sim 0.06^\circ\).

The rocking-curve map of the 2-in. wafer at \(\phi = 0^\circ\) is shown in Fig. 2(a). Here, the incident-beam direction is anti-parallel to the \(x\)-direction, as indicated by the purple arrow in Fig. 2(a). Line profiles of the three areas marked in Fig. 2(a) are shown in Fig. 2(c) with their polynomial fits (red lines). The high-frequency signals may originate from the dotted pattern of the GaN films and substrate. Dotted patterns were employed on the GaN substrate to minimize the lattice mismatch and strain during the crystal growth. The angle deviation started to increase at the edge of the sample and continued to increase until the \(x\)-direction position was approximately 2 cm. After reaching its maximum value, it decreased until reaching the end of the substrate. The angle deviation at the azimuthal angle was approximately \(\pm 0.01^\circ\). The estimated radius of curvature using this angle deviation was approximately 140 m for the centered line. This result originates from a lattice plane with a convex-up shape. Other azimuthal angles, such as 45 and 90°, do not satisfy the Bragg condition of GaN(1124) lattice planes in this configuration. The rocking-curve map shown in Fig. 2(b) is similar to that of \(\phi = 0^\circ\). The selected line profiles described in Fig. 2(d) are similar to \(\phi = 0^\circ\). The radius of curvature of the centered part was estimated to be approximately 140 m, which is similar to the value at \(\phi = 0^\circ\). However, these values varied if another line that cannot represent the curvature of the wafer was selected. Therefore, the overall feature of the lattice plane remained unclear. The stripe patterns observed parallel to the \(x\)-direction are attributed to noise from the FPS camera. This noise was also observed in the image of \(\phi = 0^\circ\), even though we subtracted the background signal using the dark image.

To obtain information on the orientation of the lattice planes, we used the following rotation matrix:16

\[
R(u_x, u_y, u_z, \alpha) = \begin{pmatrix}
\cos \alpha + u_z^2(1 - \cos \alpha) & u_x u_z (1 - \cos \alpha) - u_y \sin \alpha & u_x u_y (1 - \cos \alpha) + u_z \sin \alpha \\
u_x u_z (1 - \cos \alpha) + u_y \sin \alpha & \cos \alpha + u_z^2(1 - \cos \alpha) & u_y u_z (1 - \cos \alpha) - u_x \sin \alpha \\
u_x u_y (1 - \cos \alpha) - u_z \sin \alpha & u_y u_z (1 - \cos \alpha) + u_x \sin \alpha & \cos \alpha + u_z^2(1 - \cos \alpha)
\end{pmatrix}.
\]
Here, \((u_x, u_y, u_z)\) is the rotation axis with a vector length equal to 1, and \(a(x, y, \phi)\) is a deviation angle for sample rocking corresponding to the \(\theta_b(x, y, \phi) - \theta_{ave}(\phi)\) value described in Figs. 2(c) and 2(d). When \(\phi\) is changed to 120°, the \(x\)- and \(y\)-components are coupled together in accordance with the rotation matrix. We reset the \(q\) of GaN(1124) to \((00q)\) to enable decomposition of the vector components. The reciprocal space vector components \(q_x, q_y\), and \(q_z\) were derived by employing two rotation matrices with the GaN 1124 Bragg angle. Their relations were derived using the following multiplication:

\[
\begin{align*}
q_x, q_y, q_z &= R(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0, \Delta x)R(0, 1, 0, \Delta \theta)\begin{pmatrix}
0 \\
0 \\
q
\end{pmatrix}.
\end{align*}
\]

Here, \(\Delta \theta\) and \(\Delta x\) are expressed by the deviation angles \(a(x, y, 0^\circ)\) and \(a(x, y, 120^\circ)\), from the average values, respectively. At \(\phi = 0^\circ\), the rotation axis is parallel to the \(y\)-axis, which results in \(R(0, 1, 0, \Delta \theta)\), as illustrated in Fig. 3(a). Here, the GaN wafer lies on the \(x\)-\(y\) plane. At \(\phi = 120^\circ\), the unit vector of the new rotation axis \(y'\) becomes \(\sqrt{3}/2\) \(x\) \(- 3/2\) \(y\), which leads to \(R(\sqrt{3}/2, -1/2, 0, \Delta x)\), as shown in Fig. 3(b). Although these two matrices do not commute, i.e., \(AB \neq BA\), the effect is negligible for small angles. Here, \(A\) and \(B\) indicate arbitrary square matrices for the matrix \(R\). The evaluated \(q_x, q_y, q_z\) component map is presented in Fig. 4(a). The positive vector value indicates that the \(q_x\) component is rotated towards the \(x\)-direction. The evaluated \(q_y\) components gradually changed along the \(x\)-direction, which indicates that the lattice planes were inclined from the center to the edge of the substrate. This result corresponds to a change of the \(q_x\) value from \(-0.00116\) to \(0.00116\) \(\text{Å}^{-1}\) from one edge to another for \(q_{001}\), whose magnitude is \(2\pi/d_{001}\), almost normal to the sample surface. This \(q_x\) range corresponds to an angle of \(\pm 0.027^\circ\) between \(q_x\) and \(q_z\). The calculated \(q_x\) values indicate that the crystalline films were inclined and wavy at the edge of the substrate. We applied this calculation to the \(q_x\) direction shown in Fig. 4(b). Here, the positive vector indicates that the GaN(0001) lattice planes were rotated towards the \(x\)-direction. The calculated \(q_x\) values gradually changed along the \(y\)-direction, which implies that the lattice plane was almost flat in the \(y\)-direction of the investigated wafer. The calculated angle between the \(q_x\) and \(q_y\) vectors was approximately \(\pm 0.01^\circ\), which is significantly smaller than the value obtained from the \(q_x\) information. This finding is attributed to the GaN(0001) lattice planes of the substrate with an almost cylindrical shape having one-directional curvature similar to cleaved firewood. It is noted that X-ray miscut-angle measurements for a wafer prepared by the same company using the same growth method were not contradictory. If the GaN(0001) lattice planes had a spherical shape, similar to a concave or convex lens, the \(q_x\) and \(q_y\) distributions would be homogeneous in all directions. The blue line in the diagonal direction in Fig. 4(b) from the top-left to bottom-right originates from dead FDS pixels. To better visualize the lattice planes, we projected the vector \(q_x, q_y, q_z\) components onto the \(x\)-\(y\) plane, as shown in Fig. 4(c). We reduced the total data points to 1/20 to better visualize the vector in the \(x\)-\(y\) plane because it is difficult to see all the vector components in the specified area. The evaluated vector arrows mostly point towards the outside of the substrate from the center line. The short arrow length indicates that the vector components in the \(q_x\) or \(q_y\) direction are small and that the crystal plane is almost perpendicular to the \(z\)-direction, as shown in Figs. 4(d) and 4(e). The inclination of the lattice towards the \(x\)-direction is far more dominant than that towards the \(y\)-direction. We calculated the length of the vector components \(q_x, q_y, q_z\) as shown in Fig. 4(d). The results indicate that the central, top, and bottom parts had low values. The blue areas represent regions where there are almost no \(q_x\) or \(q_y\) components, and the red areas represent regions where \(q_x\) or \(q_z\) components exist. Near the positions of \((x, y) = (2\text{ cm}, 4\text{ cm})\) and \((4.5\text{ cm}, 3\text{ cm})\), lattice-plane inclination to the left and right
directions is observed, which provides further evidence of the cylindrical shape of the (0001) lattice planes.

These results are far more informative than those presented in Fig. 2, which merely show some curvature-like information in one direction. To confirm the lattice orientation, it was imperative to introduce a rotation matrix. Even though stripe patterns were observed in the evaluated images in the diagonal direction, these patterns were attributed to FPS noise rather than the sample structure. The stripe patterns in Figs. 2(a) and 2(c) affected the matrix operation, which also generated stripe patterns in the reciprocal lattice vector $q$.

In addition, we evaluated the tilt-angle distribution (shown in Fig. 5) using the polar angles of all the $q$ vectors in Fig. 4(c). The obtained full width at half maximum was $0.0156^\circ$. The origin of the centered area in the distribution comes from the relatively flat parts of the lattice plane. On the other hand, the tilting angles above the central area arise mainly from the relatively large curvatures around the edges of the sample wafer.

According to recent research on the lattice-plane bending of the a 4H-SiC substrate, the overall shape of the lattice planes can be estimated by measuring one-directional rocking curves at some points of the SiC wafer.\(^5\) Even though this method provides information on the overall shape of the lattice planes, it does not provide information on the direction of the reciprocal vector components $q_x, q_y, q_z$. Similar methods were suggested by Mikulík\(^{17}\) and Lübbert\(^{18}\), however, they did not introduce a rotation matrix in the image reconstruction to obtain the $q_x, q_y, q_z$ information for the Bragg peaks. Our method using grazing-incidence XRDT provides the direction of the lattice planes for all the positions on a sample, including the curvature of the lattice-plane orientation. In addition, this approach is effective because of the shorter data-acquisition time ($\sim$30 min), which is fast enough for adoption in wafer inspection and other applications. Even though our proposed method may only be valid for a nearly perfect crystal, it is useful to understand the lattice-plane orientation within a short time. We observed the lattice-plane tilting of the homo-epitaxial layer because the X-ray extinction length was approximately 1.3 $\mu$m smaller than the layer thickness. The main contribution may be from the substrate crystal.

In general, laser-based systems are used for monitoring the stress and curvature of a wafer according to the change of the laser spot positions. However, the reflected laser beam position provides information not on the lattice planes but rather on the surface-normal direction.

In conclusion, we proposed an XRDT-based method for observing lattice-plane directions. By measuring the X-ray diffraction at the azimuthal angles of $\phi = 0$ and 120$^\circ$ and using a rotation matrix, we obtained the $q_x$, $q_y$, and $q_z$ components of every point on a 2-in. wafer. The GaN(0001) planes evaluated from measurements using the two 1124 reflections exhibited a cylindrical shape rather than a spherical shape. This method is useful for understanding the crystal lattice-plane orientation.

**Acknowledgment** The XRDT measurements were performed at BL20B2 of SPring-8 under proposals Nos. 2017A1030, 2017A1033, 2017A4504, 2017B1029, 2017B4504, and 2017B4505. This work was supported by MEXT “Program for Research and Development of Next-Generation Semiconductor to Realize Energy-Saving Society”.

1) A. Bykhovski, B. Gelmont, and M. Shur, J. Appl. Phys. 74, 6734 (1993).
2) C. Kisselowski, J. Krüger, S. Ruvimov, T. Sasaki, J. W. Ager, III, E. Jones, Z. Liliental-Weber, M. Rubin, E. R. Weber, M. D. Bremser, and R. F. Davis, Phys. Rev. B 54, 17745 (1996).
3) A. Segmüller, J. Angeliolo, and S. J. La Placa, J. Appl. Phys. 51, 6224 (1980).
4) J. Hoizowska, A. K. Freund, E. Boller, J. P. F. Sellschop, G. Level, J. Hartwig, R. C. Burns, M. Rebak, and J. Baruchel, J. Phys. D, 34, A47 (2001).
5) Z. B. Zhao, J. Hershberger, S. M. Yalisove, and J. C. Bilello, Thin Solid Films 415, 21 (2002).
6) Y. Cui, X. Hu, X. Xie, R. Wang, and X. Xu, CrystEngComm 19, 3844 (2017).
7) W. Berg, Naturwissenschaften 19, 391 (1931) [in German].
8) R. W. Armstrong and J. M. Schultz, Surf. Sci. 12, 19 (1968).
9) S. Nakamura, T. Mukai, and M. Senoh, Appl. Phys. Lett. 64, 1687 (1994).
10) A. Reiher, J. Bässing, A. Dadgar, A. Diez, and A. Krost, J. Cryst. Growth 248, 563 (2003).
11) I. A. Buyanova, J. P. Bergman, B. Monemar, H. Amano, and I. Akasaki, Appl. Phys. Lett. 69, 1255 (1996).
12) M. Städele, J. A. Majewski, and P. Vogl, Phys. Rev. B 56, 6911 (1997).
13) X. H. Wu, P. Fini, E. J. Tarsa, B. Heying, S. Keller, U. K. Mishra, S. P. DenBaars, and J. S. Speck, J. Cryst. Growth 189–190, 231 (1998).
14) A. Usui, H. Sunakawa, A. Sakai, and A. A. Yamaguchi, Jpn. J. Appl. Phys. 36, L899 (1997).
15) S. Takashima, K. Ueno, H. Matsuyama, T. Inamoto, M. Edo, T. Takahashi, M. Shimizu, and K. Nakagawa, Appl. Phys. Express 10, 120004 (2017).
16) D. J. Huggins, J. Comput. Chem. 35, 377 (2014).
17) P. Mikulík, D. Lübbert, D. Kortýr, P. Pernot, and T. Baumbach, J. Phys. D 36, A74 (2003).
18) D. Lübbert, C. Ferrari, P. Mikulík, P. Pernot, L. Helfen, N. Verdi, D. Kortýr, and T. Baumbach, J. Appl. Crystallogr. 38, 91 (2005).