Local lattice-plane orientation mapping of 6-inch GaN wafer using X-ray diffraction topography

X-ray diffraction topography (XRDT) has a long history. Many methods of XRDT were derived and modified in laboratories and in synchrotron X-ray facilities. Various books for understanding the methods and reviews of their historical developments, for example [1], can be found so we do not explain the details of XRDT here. Such XRDT techniques have been helpful for visualizing crystal imperfections such as extended defects, dislocations, and stacking faults. Accordingly, from an industrial viewpoint, the methods have provided feedback for improving the crystallinity, or crystal perfection, to develop silicon (Si), III-V, oxide, wide-bandgap crystals, and so on.

The authors proposed a modified XRDT method [2] to map local lattice-plane orientation, that is, to visualize the local lattice-plane shape of a whole wafer. The method records rocking curves around a Bragg condition from a whole wafer using a monochromatic and sufficiently large X-ray beam and an X-ray two-dimensional (2D) detector for two reflections without sample translation, enabling us to perform a simple measurement compared with one using a small beam and requiring sample translation. Many reports regarding synchrotron X-ray diffraction imaging have discussed sample crystallinity in terms of diffracted intensities, rocking-curve widths, and peak positions. A few research groups, however, have discussed the lattice-plane shape using rocking curves from selected sparse positions along several directions [3].

Applying the method to the visualization of a local lattice shape, our group has intensively studied c-plane 2-inch and 4-inch GaN wafers and an m-plane substrate as well as their homoepitaxial thin films. Several of our articles have been cited not only to introduce the results, but also to explain the concept behind our proposed method and the application limitations related to a local d spacing and a local lattice-plane curvature [4].

Next, we present the key point of the concept. We use center angular positions of rocking curves from many positions on a sample surface with a 2D detector and evaluate local deviation angles on two respective diffraction planes. Local reciprocal-lattice (q) vectors for respective sample surface positions are evaluated using the deviation angles via the rotation matrix.

Let us also introduce an example of information obtained from the 4-inch wafer. The q vector components evaluated from the two rocking-curve images at different azimuthal angles combined with the rotation matrix revealed that overall lattice planes bowed towards the diagonal direction.

We here introduce the synchrotron X-ray diffraction characterization results of a 6-inch free-standing GaN (0001) wafer grown using a Na-flux-based LPE method and the crystallinity and local lattice plane shape of the whole wafer [5]. The crystallinity and local lattice plane shape of the whole wafer were discussed using the maps of $11\bar{2}4$ peak intensities and the rocking curve FWHM widths for the two azimuthal angles ϕ = 0 and 120°. In addition, the local q vector maps were visualized. The following findings were obtained. 1) Huge boundaries were observed between the high- and low-crystallinity areas. 2) The lattice plane was observed to be anisotropically bowed along

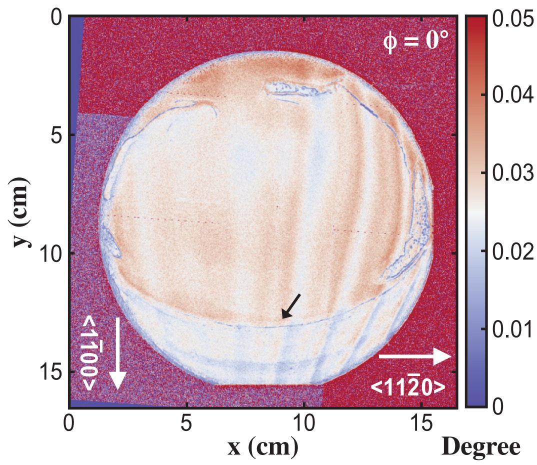

Fig. 1. X-ray diffraction topography images reconstructed from the rocking curve width. The higher crystalline area (blue) and lower crystalline area (red) are separated by the border in the substrate bottom. The undulation of the FWHM along the X-ray direction on the substrate is seen at ϕ = 0°. [5]

the [10$\bar{1}$0] direction. 3) The mean width of the rocking curves over the wafer was 0.024°.

An X-ray diffraction topography measurement was performed at SPring-8 **BL20B2**. X-rays of 1.3 Å were chosen and the X-ray beam size was adjusted to be larger than 100 mm (h) × 3 mm (v). Because of the limitation of the detection area of a flat panel detector (Hamamatsu, C7942CA-22), the 6-inch substrate was required to be translated to almost perpendicular and parallel directions with respect to the X-ray incident beam to achieve full-area illumination. The detector was placed almost parallel to the sample surface with a sample-to-detector distance of 30 cm. The detector pixel size was 50 × 50 μm^2, and the pixel numbers were 2368 × 2240. The 6-inch substrate was placed at the rotation center by minimizing tension. The interplanar angle between GaN (0001) and (11$\bar{2}$4) is 39.16°, and the 11$\bar{2}$4 Bragg angle was 40.25°, resulting in an incident angle of about 1°, which was small enough to cover the whole substrate. Under this asymmetric X-ray illumination, the X-ray incident angle was scanned using 5 arcsec steps. The X-ray exposure time was 5 s, and more than 2000 diffracted images were recorded at the fixed azimuthal angle ϕ.

The FWHM map of the 6-inch free-standing GaN substrate at ϕ = 0° is illustrated in Fig. 1. Striped lines are seen along the [10$\bar{1}$0] direction. The value at the substrate edge area at the top is higher than those in other places. Around the substrate bottom below the border, the FWHM is even smaller than that at the substrate center, which indicates a localized higher crystallinity area. We attribute this to strain relaxation followed by dislocation formation. It is known that the strain of a free-standing GaN crystal is dependent on the GaN thickness on foreign substrates. Therefore, during the crystal growth or laser lift-off process, some parts in the substrate may be strained so that the substrate undergoes local deformation. Although the mechanism of this phenomenon remains unclear, substrate bending and dislocation may provide a plausible explanation that may be related to the striped FWHM patterns. The same analysis was conducted at ϕ = 120° (not shown here). The overall features appear similar, and the stripe patterns are inclined compared with those at ϕ = 0°. The FWHM map does not change continuously on the borderline around the substrate bottom, indicating that the substrate has already deformed along the boundary.

To evaluate the 2D lattice-plane tilting, we analyzed the local q-vectors of GaN 11$\bar{2}$4. The q-vector analysis method is described elsewhere [2]. Two rotation matrices for the calculation of the angular change of the q vector were introduced. The projection of the q vector to the (x, y)-plane is depicted in Fig. 2(a). In the vector plot, the direction of the arrow indicates 2D inclination with respect to the mean lattice-plane bending angle. In particular, for the left and the right sides, the lattice plane moved significantly toward the substrate center. Interestingly, substrate bending from top to bottom is much less than that in other directions. Figure 2(b) shows the amplitude of the projected vector in Fig. 2(a) and indicates cylindrical bowing.

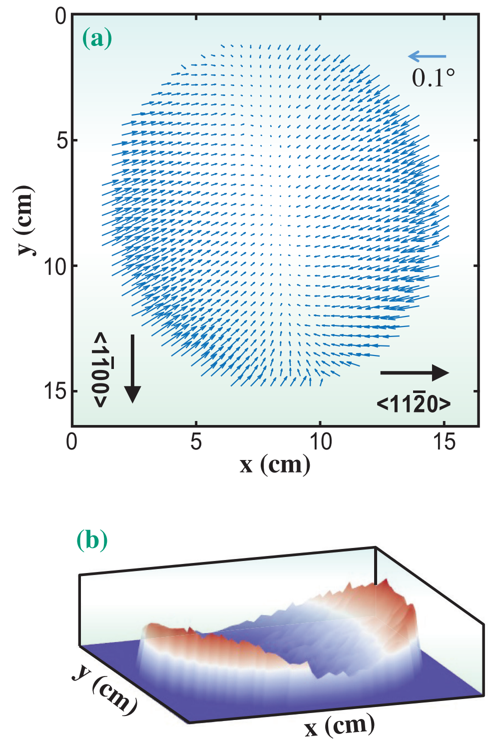

Fig. 2. **(a)** Lattice plane bending direction projected to the (x, y)-plane. Symmetrical substrate bending with respect to the y-direction is observed. **(b)** Degree of substrate bending visualized from the magnitude of projected vectors. [5]

Osami Sakata[a,*] and Jaemyung Kim[b]

[a] Japan Synchrotron Radiation Research Institute (JASRI)
[b] RIKEN SPring-8 Center

*Email: sakata.osami@spring8.or.jp

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