# Anomalous lattice deformation in GaN / SiC(0001) measured by *in situ* synchrotron X-ray diffraction

Gallium nitride (GaN) is widely used for LEDs and high-frequency power devices and has the potential to drastically reduce power consumption beyond what has been achieved by conventional materials such as silicon (Si) or gallium arsenide (GaAs). Thus, the more widespread use of GaN-based devices is expected to help realize a future low-energy society. Despite these technological advances, many issues affecting the crystal growth of GaN still remain. For example, the lattice deformation of GaN in the initial growth stage has not been fully clarified. In the case of GaN/SiC(0001) heteroepitaxy, this property should be characterized at the growth temperature because of a large thermal mismatch between the film and the substrate, which would induce large state variations during cooling [1]. Reflection high-energy electron diffraction (RHEED) is commonly used for *in situ* monitoring in molecular beam epitaxy (MBE), and the surface morphology can be evaluated from changes in the RHEED pattern or intensity [2]. Furthermore, this technique can provide the lattice parameter along the in-plane direction, which is estimated from the spacing between streaks [3]. However, conventional *in situ* monitoring is insensitive to the lattice parameter along the surface normal direction, knowledge of which is necessary to estimate the lattice deformation more precisely. In this study, *in situ* synchrotron X-ray diffraction (*in situ* XRD) was conducted to measure the lattice parameters of GaN in both the in-plane and out-of-plane directions. The combined use of a high-brilliance synchrotron radiation source and a two-dimensional (2D) detector has enabled high-speed measurements with atomic-scale resolution. Using this method, we found anomalous lattice deformation during the initial growth of GaN, and a new deformation model that defies conventional theory was proposed.

Experiments were performed at SPring-8 **BL11XU** using a plasma-assisted MBE system that is directly coupled to an X-ray diffractometer [4]. In the MBE chamber, following the removal of native oxides from the Si-faced 6H-SiC(0001) substrate by high-temperature heating, GaN was directly grown on the substrates as shown in Fig. 1. X-rays with the energy of 20 keV were focused to a size of $0.1 \times 0.1$ mm$^2$ by a four-blade slit. The diffracted X-ray signals were detected by a 2D detector (PILATUS 100K) with an angular resolution of 0.014°.

Figure 2 shows typical obtained experimental data. The diffraction peak of GaN-101 was confirmed to emerge as the thickness of the GaN film reached 0.8 nm, corresponding to approximately two atomic layers. This means that our real-time measurement is quite effective for evaluating lattice deformation quantitatively at the atomic layer scale.

Figure 3 shows film-thickness dependences of the diffraction-peak positions along the out-of-plane (L) and in-plane (H) directions. These positions are related to the reciprocal of the lattice spacing of GaN in each direction. In the conventional strain relaxation of crystals, the lattice spacing in the L-direction changes in conjunction with that in the H-direction. That is, when a film with a larger lattice constant than the substrate is relaxed, the rate of decrease in the lattice spacing along the L-direction is almost identical to the rate of increase along the H-direction; this is known as conventional elastic theory. However, Fig. 3 shows that the variation in the H-direction is small compared with that in the L-direction. In order to understand this anomalous phenomenon, a new

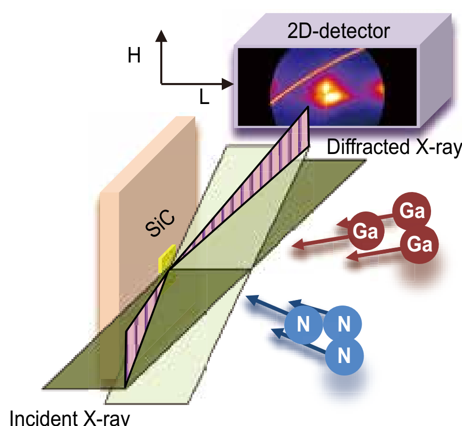


Fig. 1. Schematic of *in situ* XRD during the growth of GaN on a SiC substrate.

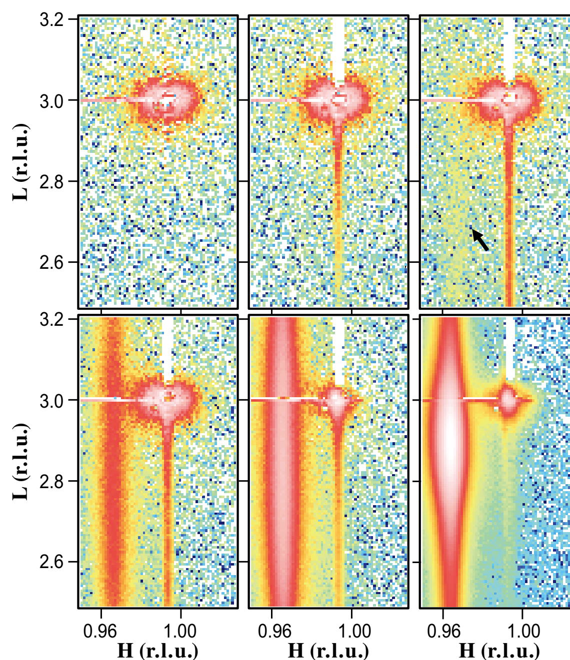


Fig. 2. Typical reciprocal space maps obtained by *in situ* XRD. The GaN thicknesses are 0 (before growth), 0.5, 0.8, 1.0, 2.1, and 10 nm. With increasing GaN film thickness, the diffraction peak of GaN becomes larger and its peak position is gradually shifted.

lattice-deformation model reflecting lattice expansion due to the incorporation of point defects (Ga anti-site defects) was considered, leading to a good fitting with the experimental data as shown by the calculation result in Fig. 3. This suggests that depending on the growth condition, many more point defects than are expected can be incorporated into the GaN film [5].

We have proposed the new lattice-deformation model of the GaN film on the basis of the results of real-time observation. Since this model is important for controlling the point-defect density in GaN, it is expected to optimize the growth conditions for GaN films with high quality and a low defect density in the future.

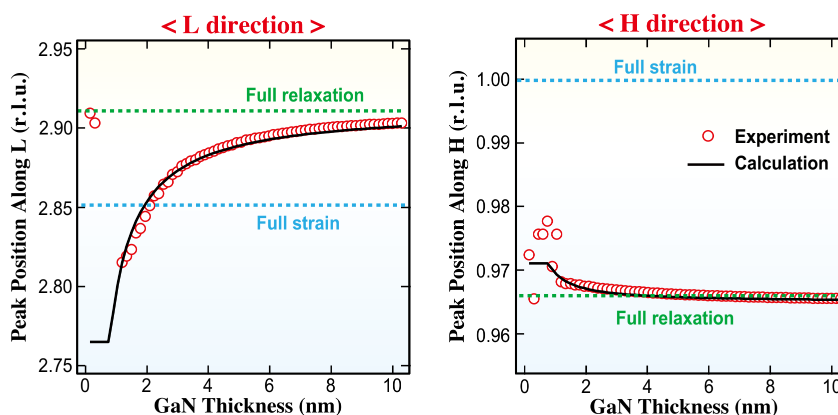


Fig. 3. Film-thickness dependences of the peak positions. It is clear that the lattice spacing along the L-direction shifted more than that along the H-direction, indicating a difference from conventional elastic theory. "r.l.u." indicates reciprocal lattice unit and a large (small) value corresponds to a small (large) lattice spacing of GaN.

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**Reference**

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