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# Analysis of Inclined Threading Dislocation from GaN [0001] by Raman mapping

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## Abstract

Threading dislocations (TDs) in GaN single crystal is analyzed by Raman mapping image of  $E_2^H$  peak shift. While large number of black-and-white dot contrasts occupy the mapping area, a black-and-white streak contrast along  $[\bar{1}\bar{1}20]$  direction is also observed. The location of the streak contrast agrees between Raman mapping image and X-ray topography image. The streak contrast is considered to be the presence of a strain field spreading in the  $[\bar{1}\bar{1}20]$  direction in the GaN crystal. The computer simulation of the Raman mapping image reveals that the TD is inclined from [0001] toward  $[\bar{1}\bar{1}20]$ . It is found that not only the distribution and type but also the inclined direction and angle of TDs from the *c*-axis GaN can be measured by Raman spectroscopy.

## 1. Introduction

GaN is expected as a power device material because of its excellent physical properties. Threading dislocation (TD) analysis in a freestanding GaN substrate is important because it affects device characteristics. Several evaluation methods for TDs in GaN crystals, such as chemical etching, transmission electron microscopy, X-ray topography, cathodoluminescence, and photoluminescence, are proposed<sup>[1]</sup>. However, it is not easy to detect and classify the TDs by nondestructive at laboratory-scale. In previous work, we have succeeded in detection of edge-component TDs in GaN using Raman spectroscopy<sup>[2]</sup>. Raman spectroscopy is a nondestructive, laboratory-scale instrument that can measure the strain field of TDs. In the Raman mapping image of  $E_2^H$  peak shift in *c*-plane GaN, black-and-white dot contrasts due to TDs were observed. The density, in-plane direction, and magnitude of the edge-component of the TDs were determined<sup>[3]</sup>. In this study, we investigated the black-and-white streak contrast that is stretched in one direction.

## 2. Experimental

A free-standing *c*-plane GaN substrate, grown by hydride vapor-phase epitaxy, was used for the evaluation sample. The

thickness and density of the TDs were 350  $\mu$ m and ~10<sup>5</sup> cm<sup>-2</sup>, respectively. Raman scattering spectroscopy measurements were performed at RT using an in-Via Raman system (REN-ISHAW)<sup>[2],[3]</sup>. To increase the wavenumber resolution, the 532 nm laser intensity was maximized ~150 mW and the grating width of 3000 gl/mm was selected. An objective lens with a magnification of 100 times and a high numerical aperture (NA) of 0.85 were used. The irradiation time and integration number were 0.2 s and 1, respectively. A step width of 0.3  $\mu$ m was applied to increase the spatial resolution. The wavenumber resolution at the detector was estimated to be 0.8 cm<sup>-1</sup>. For data analysis, the Raman software WiRE 3.4 (made by RENISHAW) was used.

In the Raman mapping simulation, it was assumed that a 20  $\mu$ m square range containing one TD (Fig.1). Here, calculation was performed on the assumption that Raman scattering in the laser irradiation region is dominant. The irradiation area was a three-dimensional area in the range of the focal depth, and the light path was in line with the shape of the Gaussian beam, and the irradiation area of the laser was determined. The calculation of Raman mapping is based on the theory of elasticity<sup>[4]</sup>. The E<sub>2</sub><sup>H</sup> peak shift ( $\Delta \omega_{E_2^H}$ ) in Raman scattering is expressed by the following equations:

$$\Delta \omega_{\rm E_2^{\rm H}} = a_{\rm E_2^{\rm H}} (\varepsilon_{xx} + \varepsilon_{yy}) + b_{\rm E_2^{\rm H}} \varepsilon_{zz}, \qquad (1)$$

Here, the deformation potential constants of  $a_{E_2^H} = -850 \text{ (cm}^{-1})$ ,  $b_{E_2^H} = -920 \text{ (cm}^{-1})$  were used<sup>[5]</sup>.

X-ray topography was conducted at the beam line of BL8S2 in Aichi Synchrotron Optical Center. The diffracted X-rays were imaged on a nuclear dry plate. In X-ray topography, the diffraction planes of  $g = (\overline{1124})$  was used.

#### 3. Results and discussions

Figure 2 (a) shows Raman mapping image of  $E_2^H$  peak shift in GaN. The mapping image of  $E_2^H$  peak shift of GaN exhibits the pairs of higher and lower wavenumber regions, which correspond to the compressive and tensile strains due to TDs. Clear black-and-white dot contrasts were observed

more than 10 in  $100 \times 100 \ \mu\text{m}^2$  area. Further, a black-andwhite streak contrast extending in the  $[\overline{1}\overline{1}20]$  direction near the center area (shown by the red square frame). This is considered to be the presence of a strain field spreading in the  $[\overline{1}\overline{1}20]$  direction in the GaN crystal. The X-ray topography image of the same location (Fig. 2 (b)), a weak contrast is also observed. Judging from the Raman mapping and X-ray topography image, it can be estimated that the TD has a large inclination from the *c*-axis direction.

The Raman mapping contrast of  $E_2^H$  peak shift was created by computer simulation. Figure 3 (a) shows an enlarged experimental Raman mapping image of the area from fig. 2 (a). Figure 3 (b)-(d) shows simulated Raman mapping image of  $E_2^H$  peak shift containing a TD with inclined from the *c*axis toward the [ $\overline{1120}$ ]. The inclination angle was 0°, 30°, and 60°, respectively. By increasing the inclination angle, the black-and-white contrast was expanded toward the [ $\overline{1120}$ ] direction. In addition, the contrast with 60° became weaker than that with 0° or 30°. We thus conclude that the streak contrast in the Raman mapping image is attributed to the inclined TD from the *c*-axis direction.



Fig. 1 Schematic of simulation model for Raman mapping.







Fig. 3 (a) Enlarged image of red square area from fig. 2(a). Simulated Raman mapping images of  $E_2^{H}$  peak shift assuming threading edge dislocations with inclination angle of (b) 0°, (c) 30° and (d) 60° from [0001].

# 4. Conclusions

We analyzed TDs in a HVPE-grown *c*-plane (0001) GaN single crystal by micro Raman spectroscopy mapping. While large number of black-and-white dot contrasts occupy the mapping area, a black-and-white streak contrast along  $[\bar{1}\bar{1}20]$  direction is also observed. The location of the streak contrast agrees between Raman mapping image and X-ray topography image. The streak contrast is considered to be the presence of a strain field spreading in the  $[\bar{1}\bar{1}20]$  direction in the GaN crystal. The computer simulation of the Raman mapping image reveals that the TD is inclined from [0001] toward  $[\bar{1}\bar{1}20]$ . It is found that not only the distribution and type but also the inclined direction and angle of TDs from the *c*-axis GaN can be measured by Raman spectroscopy.

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