X-ray Diffraction Analysis of Threading Dislocations in GaN Thin Films

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Motivation—In recent years, GaN has emerged as an attractive new material for optoelectronic and electronic device applications. The wide bandgap of GaN and its alloys enables light-emitting devices with wavelengths spanning the green, blue, violet, and ultra-violet (UV) regimes. Potential applications for these light emitters include efficient solid-state lighting for buildings and UV-based detection of biological agents. The high breakdown field and high mobility of GaN also enables high-speed, high-power transistors operating at frequencies near 10 GHz. These transistors are suitable for making lightweight, compact power-supplies for phased-array synthetic aperture radars. All of these applications use GaN thin films grown on sapphire or SiC substrates. Since heteroepitaxy of GaN on these lattice-mismatched substrates remains challenging, these films contain numerous threading-dislocation defects that limit device performance and lifetime. Thus, convenient methods for accurately measuring the threading-dislocation density are needed to support ongoing work to improve the GaN film quality and to assess the impact of dislocations on device performance.

Accomplishment—We have developed an improved x-ray diffraction (XRD) method for measuring the threading-dislocation density in GaN thin films. The method rests on the fact that the strain fields produced by dislocations cause both inhomogeneous tilting and twisting of the GaN crystal planes and localized incoherence of the crystal lattice. As shown in Fig. 1, these real-space distortions lead to corresponding broadening of the reciprocal-lattice points of the crystal. XRD systematically probes this broadening by measuring the characteristic width of selected Bragg-diffraction peaks. The (*hkl*) dependence of the peak-width broadening is interpreted using a reciprocal-space model that convolves the tilt variance, the twist variance, and the coherence length of the dislocated film. Fitting of the model to experiment uniquely deconvolves the tilt, twist, and coherence-length contributions. The threading-dislocation density then follows using previously developed dislocation theory that relates the deconvolved lattice rotations to the dislocation density. The resultant threading-dislocation density has been benchmarked against transmission electron microscopy (TEM); good agreement is found. Recently, the validated XRD technique was used to measure the threading-dislocation density in high-electron-mobility transistors (HEMTs) with room-temperature mobilities ranging from 231 to 1830 cm^2/V-s. In Fig. 2, we compare the HEMT mobility to the measured dislocation density and find that mobility tends to decrease as dislocation density increases. Importantly, high mobility (> 1800 cm^2/V-s) occurs at low threading-dislocation density (< $1x10^9$ cm^{-2}).

Significance—The XRD method for measuring dislocations has several key advantages. First, unlike TEM, no destructive and time-consuming sample preparation is required. Second, a large sample area is probed; this eliminates point-sampling errors inherent to all microscopy-based methods. Finally, unlike most methods, both low (~$1x10^8$ cm^{-2}) and high (~$1x10^{11}$ cm^{-2}) dislocation-density samples are probed with nearly equal ease. Because of these advantages, XRD measurements of threading-dislocation density are increasingly used to support the development of GaN-related materials and devices at Sandia.

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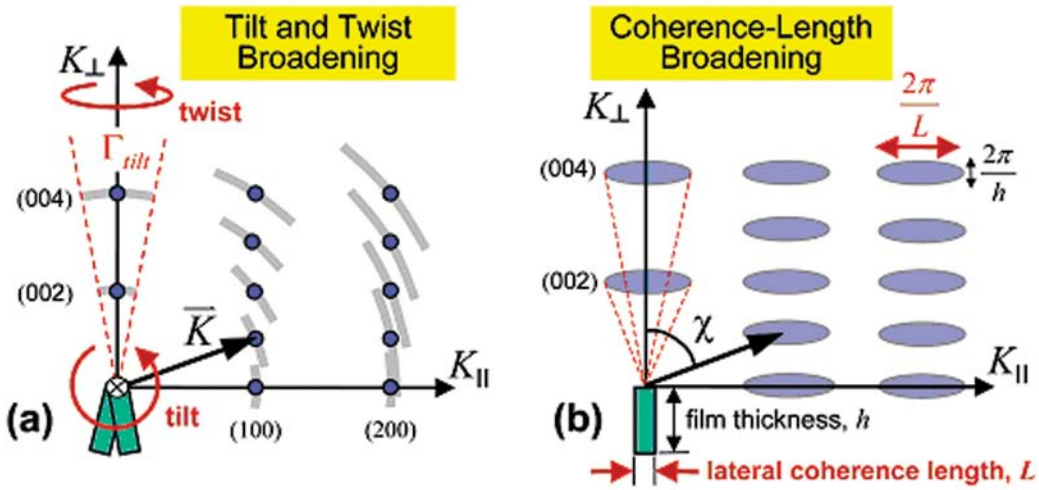

$$\textbf{(c)}\quad \Gamma_{hkl}^2 = \left(\Gamma_{tilt}\cos\chi_{hkl}\right)^2 + \left(\Gamma_{twist}\sin\chi_{hkl}\right)^2 + \left(2\pi/L\right)^2/\left|K_{hkl}\right|^2$$

Figure 1. (a) Variations in the tilt and twist orientation of local domains in the GaN epilayer (*green rectangles*) cause purely transverse broadening of the reciprocal lattice (*blue dots*). (b) The finite size of the domains causes additional non-transverse broadening of the reciprocal lattice (*blue ellipses*). (c) Convolution of the broadening contributions due to tilt, twist, and coherence length yields the total peak width, Γ_{hkl}, at each reciprocal-lattice point.

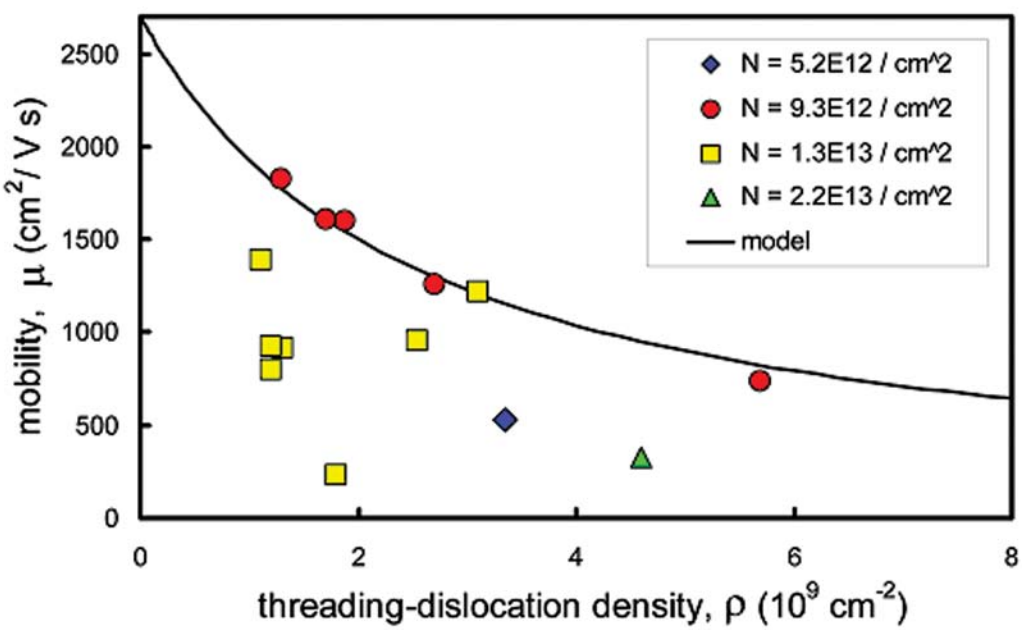

Figure 2. Room-temperature 2-D electron-gas mobility versus threading-dislocation density for GaN-based HEMTs. In the legend, **N** is the sheet-carrier density of the 2-D gas. The model has the form $1/\mu = 1/\mu_p + 1/\mu_d$, where $\mu_p = 2700$ cm^2/Vs is the optical-phonon contribution, $\mu_d = C/\rho$ is a dislocation-related scattering contribution, and C is a fitting parameter. Downward deviations from the model may be due to additional scattering produced by roughness at the AlGaN/GaN interface.