Epitaxial Tilting of GaN Grown on Vicinal Surfaces of Sapphire

X.R. Huang[1], J. Bai[1], M. Dudley[1], R.D. Dupuis[2], and U. Chowdhury[2]

[1]Department of Materials Science and Engineering, Stony Brook University; [2]School of Electrical and Computer Engineering, Georgia Institute of Technology

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For More Information
Michael Dudley, Department of Materials Science and Engineering, Stony Brook University

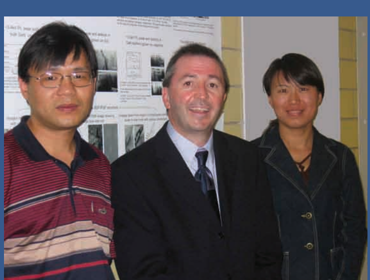
Email: mdudley@notes.cc.sunysb.edu

Using the synchrotron Laue method and high-resolution x-ray diffraction, we have revealed the epitaxial tilting effect of gallium nitrite (GaN) films grown on vicinal (0001) surfaces of sapphire and their relationship to the offcut angles and the substrate surface steps. This effect is a consequence of the large out-of-plane lattice mismatch between GaN and sapphire, and can be explained by an extended Nagai theory. The large lattice tilts and their formation mechanism indicate that the substrate surface morphology is an important factor that affects the epitaxy process and the crystalline quality of GaN films grown via vicinal-surface epitaxy.

Although the growth of III-nitrides on sapphire (Al_2O_3) has been extensively investigated, little attention has been paid on the large *c* lattice mismatch ($\Delta c/c \approx$ 20% for GaN/sapphire), particularly the case of vicinal surface epitaxy (VSE). We have recently demonstrated that GaN grown on a vicinal sapphire surface is generally tilted from the substrate (known as a Nagai tilt). For 1-bilayer steps of sapphire, shown in **Figure 1a**, the tilt α is related to the offcut angle φ by the relationship $\tan\alpha = -(\Delta c/c)\tan\varphi \approx 0.2\tan\varphi$ (<0). For step bunches, however, this principle may change. In **Figure 1c**, due to $3c \approx 2.5c_e$, the GaN lattices can be tilted in two directions with equal probabilities, $\tan\alpha \approx \pm 0.2 \tan\varphi$, leading to $\alpha \approx 0$ on average. For 4-bilayer steps, the GaN lattice is tilted *toward* the offcut direction by $\tan\alpha = [(4c-3c_e)/(4c)]\tan\varphi \approx 0.1 \tan\varphi$ (>0). Similarly, the tilt for 5-bilayer steps is $\tan\alpha = [(5c-4c_e)/(5c)]\tan\varphi \approx 0.04 \tan\varphi$ (>0).

The above principles have been explicitly verified by synchrotron Laue patterns and high-resolution x-ray diffraction performed on vicinal GaN/sapphire. GaN films 4 μm thick were grown using low-pressure metal organic chemical vapor deposition (MOCVD) in a temperature range of 1020-1080°C. **Figure 2** shows the back-reflection Laue patterns of three samples, where the displacement of the 0001 spot from *O* (white arrows) is caused by the offcut, and the displacement of the GaN 0001 spot from that of sapphire reflects the epilayer tilt, which is always parallel to the offcut direction $\mathbf{n}_c$. In **Figure 2a**, the measured tilt (negative) is in perfect agreement with the tilting model in **Figures 1a** and **1b**, indicating that on the small-offcut substrate the steps are dominantly 1- or 2-bilayer steps. For the 6.29°-off sample, the tilt shows that steps of various types coexist on the substrate surface, with 1- or 2-bilayer steps contributing to negative tilts and the other types reducing this tendency. The positive tilt of the 10.6°-off sample shows that 4- or 5-bilayer steps outweigh the other steps.

The tilting effect reveals a series of important mechanisms of GaN epitaxy that have been widely ignored in the past, including: 1) the sapphire surface morphology can greatly affect the epitaxy process and the crystalline quality of GaN films; 2) drastic step bunching and faceting of sapphire can occur during nitridation; 3) mismatch strains are dominantly relaxed by pure basal plane dislocations without out-of-plane Burgers vector components; and 4) the epilayer tilt-related shear stresses are believed to significantly affect the



Authors (from left) Xian-Rong Huang, Michael Dudley, and Jie Bai growth kinetics and strain relaxation. In our latest work, we also found the tilting effect and the related mechanisms in GaN/SiC systems [X.R. Huang *et al.*, PRL **95**, 086101 (2005)] where, compared to flat-surface epitaxy, VSE shows explicit advantages for relaxing strains and improving epilayer quality.

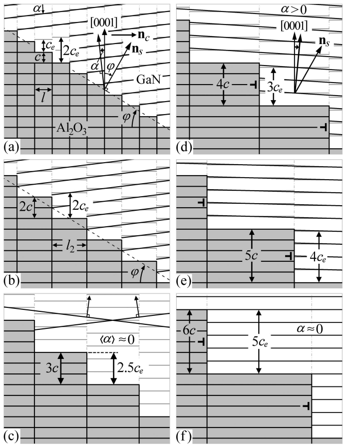


Figure 1. Epilayer tilts induced by steps of various heights in VSE of GaN on sapphire. $\mathbf{n}_s$ – substrate surface normal, $\mathbf{n}_c$ – offcut direction.

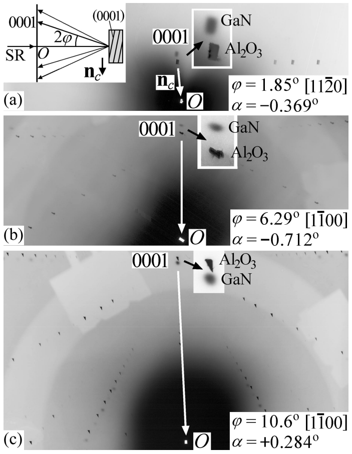


Figure 2. Laser-guided back-reflection synchrotron Laue patterns of vicinal GaN/Al_2O_3 samples showing the epitaxial tilts. The film-to-sample distance is 30 cm. Inset: a side view of the diffraction geometry.