Residual effects in GaN nanowires on ZrN buffer layers studied by XRD and Raman spectroscopy

Aleksandra Wierzbicka[1], Radoslaw Szymon[2], Eunika Zielony[2], Zbigniew R Zytkiewicz[1], Marta Sobanska Hab.[1]

[1] *Institute of Physics, Polish Academy of Sciences, Poland*
[2] *Department of Experimental Physics, Wroclaw University of Science and Technology, Poland*

Presentation type: Oral **Presentation time:** 11:15-11:30

GaN nanowires (NWs) grown on conductive transition-metal nitride buffer layers are promising for optoelectronic and electronic applications, where structural perfection and crystalline alignment are crucial for device performance. In this work, we investigate the structural properties of GaN NW ensembles grown on two different substrates: 40 nm ZrN on Si (111) and 100 nm ZrN on Al2O3 (0001). The study combines scanning electron microscopy (SEM), high-resolution X-ray diffraction (HRXRD), reciprocal space mapping (RSM), Williamson–Hall plots (W–H) analysis, and Raman spectroscopy.

The structural characterization was performed using symmetrical GaN 0002, 0004, and 0006 reflections measured in ω scans, 2θ/ω scans, and reciprocal space maps [1]. Rocking curve analysis of the GaN 0002 reflection revealed unexpectedly large tilt values for both nanowire ensembles. However, these values were not fully consistent with the morphology observed by SEM, where the nanowires appeared significantly better aligned. The Williamson–Hall analysis [2] was used to distinguish between factors related to the widening caused by microstrain and those related to the effects of orientation distribution.The W–H plot approach produced substantially lower tilt values than those obtained from rocking curves directly, suggesting that residual broadening effects significantly impact the conventional HRXRD analysis of GaN NW ensembles.

Complementary Raman spectroscopy [3] performed with green laser excitation revealed the presence of the non-polar E2(high) phonon mode together with the polar A1(LO) mode. The Raman spectra also show the presence of the forbidden A1/E1(TO) modes together with quasi-transverse phonon modes. This indicates symmetry breaking and supports the conclusions derived from the X-ray diffraction analysis.

The results presented demonstrate that, when used alone, conventional rocking curve analysis may overestimate the orientational disorder of GaN nanowires due to contributions from residual broadening. Using a combination of HRXRD, Williamson–Hall plots and Raman spectroscopy allows for a more reliable evaluation of nanowire tilt and structural quality in complex nitride heterostructures.

Acknowledgments: This work was supported in part by the Polish National Science Center, Grants No. 2022/04/Y/ST7/00043 (Weave-Unisono), 2021/43/D/ST7/01936, 2025/09/X/ST11/01089 and Foundation for Polish Science (START 088.2025). The authors are grateful to M. Guziewicz for deposition of ZrN layers and A. Reszka for SEM measurements.

References

[1] A. Wierzbicka, et al., Nanotechnology 24 (2013) 035703.
[2] V.P. Klado, et al., J. Cryst. Growth 401 (2014) 347-350.
[3] E. Zielony, et al., Appl. Surf. Sci. 588 (2022) 152901.