Investigating the Structurally and Chemically Heterogeneous Interface of AlGaN on (111) TaC

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The lack of lattice matched substrates for AlGaN is the primary limitation to achieving high-performance power electronics, high-frequency electronics, and deep UV (DUV) LEDs. This substrate limitation affects both material quality, through the formation of misfit-induced threading dislocations and strain-induced phase separation, and limitations to device geometry due to resistive or insulating electrical behavior. Dislocations and phase separation prevent AlGaN from reaching its full materials potential, and in the case of semiconducting substrates the primary loss mechanism in a vertically conductive device is resistive loss in the substrate itself. Thus, AlGaN alloys could drive disruptive technology if long-standing substrate issues can be solved [1]. For $Al_xGa_{1-x}N$ there are competing effects of increasing alloy scattering, increased bandgap with increasing Al fraction, and decreasing dopant activation such that ideal compositions for power devices fall in the range $0.3 < x < 0.85$ [2]. For these compositions pseudomorphic growth on GaN and AlN is very difficult or impossible.

Recently we have reported the design of virtual substrates for $Al_xGa_{1-x}N$ epitaxy consisting of (111) TaC_x grown on sapphire substrates via RF sputtering [3]. The crystallinity is subsequently improved by face-to-face annealing. These substrates offer several opportunities to improve power electronic devices through lattice and thermal conductivity matching, high electrical conductivity, high stability, and epitaxial liftoff.

In this talk we will discuss the nucleation of AlGaN on TaC templates as performed by molecular beam epitaxy (MBE). Annealed TaC substrates show streaky-smooth reflection high-energy electron diffraction (RHEED) patterns and 6-fold rotational symmetry. The epilayers consist of $Al_xGa_{1-x}N$ in the range $0.7 < x < 1$. Using RHEED, X-ray diffraction, atomic force microscopy, and transmission electron microscopy we investigate the impact of nucleating conditions on the structure of the film and interface. During metal-rich growth we observe incommensurate RHEED features associated with laterally contracted bilayers of metal which are not observed in nitrogen-rich growth. For $Al_{0.7}Ga_{0.3}N$ we observe relaxed growth on TaC and strained growth on co-loaded AlN templates, and corresponding to this relaxed growth only the film on TaC exhibits a step-terrace structure in AFM observed as spiral hillocks.

[1] R. J. Kaplar *et al.*, "Review—Ultra-Wide-Bandgap AlGaN Power Electronic Devices," *ECS J. Solid State Sci. Technol.*, vol. 6, no. 2, p. Q3061, Dec. 2016, doi: 10.1149/2.0111702jss.

[2] M. E. Coltrin and R. J. Kaplar, "Transport and breakdown analysis for improved figure-of-merit for AlGaN power devices," *J. Appl. Phys.*, vol. 121, p. 055706, 2017, doi: 10.1063/1.4975346.

[3] D. M. Roberts, A. Norman, M. K. Miller, and M. B. Tellekamp, "Designing low-cost TaC virtual substrates for $Al_xGa_{1-x}N$ epitaxy." arXiv, Aug. 24, 2022. doi: 10.48550/arXiv.2208.11769.

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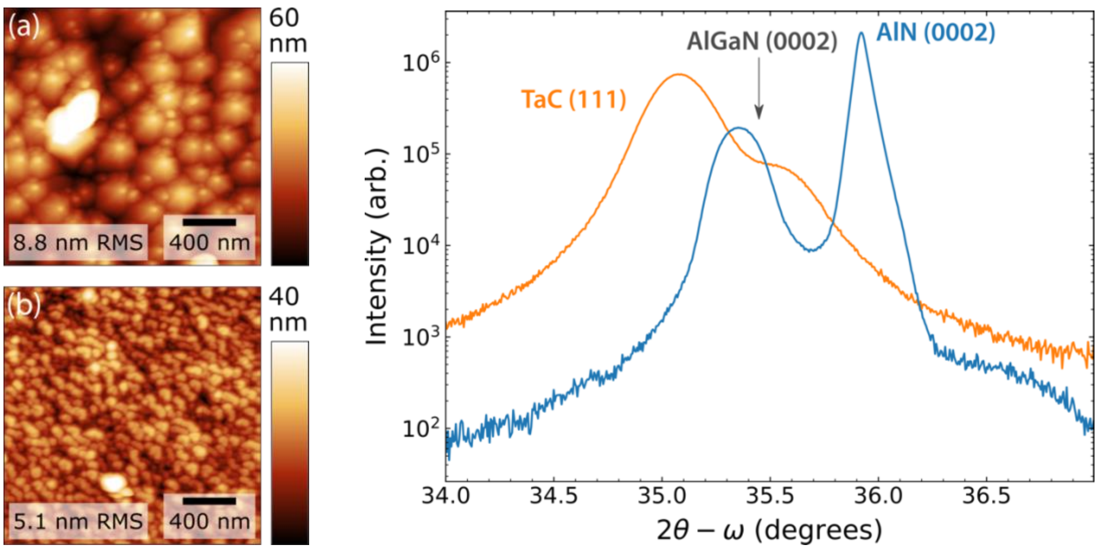
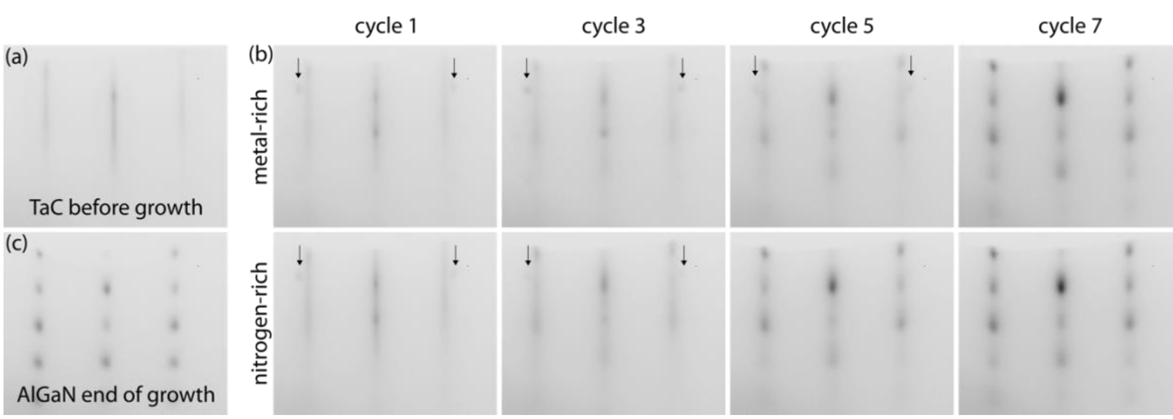
Supplemental Material



(left) AFM of $Al_{0.7}Ga_{0.3}N$ grown on TaC (a) and AlN (b) showing spiral hillocks indicative of step-flow growth and a large dislocation density. (right) X-ray diffraction of $Al_{0.7}Ga_{0.3}N$ grown on TaC and AlN



RHEED images of $Al_{0.7}Ga_{0.3}N$ nucleation on TaC. (a) shows the streaky-smooth TaC surface before growth. (b) shows RHEED captures from the first few cycles of metal-modulated epitaxy. The arrows point to an incommensurate spot which is more pronounced in metal-rich conditions and is not seen after 7 cycles. (c) shows the AlGaN at the end of growth.