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Molecular beam epitaxy of Al-Polar AlN(0001) on β-Ga₂O₃(-201)

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Research in AlN/ β -Ga₂O₃ heterostructures is driven by its potential application in transistors for power electronics. The presence of a semiconducting material with significant ionic properties like AlN offers avenues for the fabrication of hybrid devices with enhanced performance thanks to polarization effects. The existence of crystallographic planes with a reduced lattice mismatch, for instance of around 2.4% between AlN(0001) and β -Ga₂O₃(-201), is of great promise to obtain an interface with high crystalline quality.

In this study, plasma-assisted molecular beam epitaxy of AlN on bulk Fe-doped β -Ga₂O₃(-201) was performed at a substrate temperature of around 650°C, with an active nitrogen flux corresponding to the growth of 0.67 monolayers of AlN per second (ML/s) in the nitrogen-limited regime. To promote the nucleation process, the substrate was nitridated for 5 min at the growth temperature. During the nitridation process, the reflection high-energy electron diffraction (RHEED) pattern evolved from that of β -Ga₂O₃(-201) to GaN{0001}. Following the nitridation step, AlN deposition under Al-rich conditions resulted in polycrystalline growth without any preferential crystallographic texture. The resultant samples exhibited flat surface (rms surface roughness around 3.0 nm) but with brownish hue.

Additional experiments for AlN deposition were performed under nitrogen-rich conditions. In this case, the RHEED pattern smoothly evolves towards that of monocrystalline wurtzite AlN. After growth, the samples are optically transparent with an rms surface roughness below 0.5 nm. X-ray diffraction confirms the (0001) orientation of the AlN layer and reveals its epitaxial relationship with the β -Ga₂O₃(-201) substrate: Ga₂O₃ (-201) // AlN (0002) and Ga₂O₃ <020> // AlN <11-20>. Transmission electron microscopy images of the interface, coupled with energy-dispersive X-ray spectroscopy, show a sharp transition from monoclinic to wurtzite lattice, featuring an intermediate wurtzite AlGaN layer (thickness <1 nm). High-resolution images enable the identification of homogeneous Al polarity, promising for the fabrication of polarization-based nitride/oxide hybrid devices.

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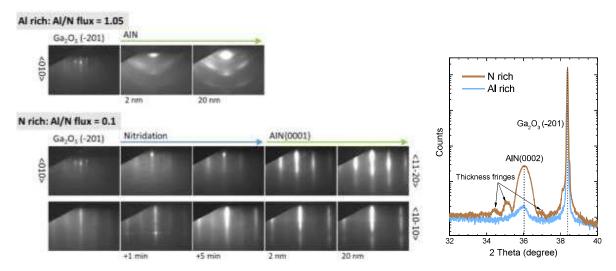


Fig. 1. Left: Evolution of the RHEED pattern during growth of AlN on β -Ga₂O₃ under Al-rich and N-rich conditions. Right: XRD θ -2 θ scan around the (-201) reflection of β -Ga₂O₃ for two 20-nm-thick AlN layers deposited under Al-rich and N-rich conditions. The layers are textured along AlN(0002). Under N-rich conditions, the improved crystalline quality enables the observation of multiple thickness fringes.

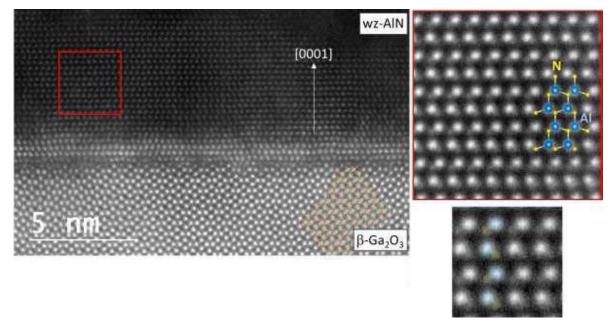


Fig. 2. High-angle annular dark field scanning transmission microscopy (HAADF-STEM) images of the AlN/Ga₂O₃ interface. The image on the left side reveals a brighter contrast at the interface on the wurtzite side. EDS measurements (not shown) confirm that the contrast arises from the presence of around 3 ML of AlGaN. Zoomed images on the right side provide unambiguous confirmation of Al polarity in the AlN layer.