

## Plasma-assisted molecular beam epitaxy of wurtzite AlN(0001) on beta-Ga<sub>2</sub>O<sub>3</sub>(-201)

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### Abstract

The realization of heterojunctions of semiconducting materials with significant ionic properties presents a fundamental interest and opens avenues for new hybrid devices with customized polarization effects. Specifically, in the case of AlN/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, research is driven by its potential application in transistors for power electronics. The formation of this heterostructure is facilitated by the existence of crystallographic planes with a reduced lattice mismatch, for instance of around 2.4% between AlN(0001) and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>(-201). In this work, plasma-assisted molecular beam epitaxy of AlN on bulk Fe-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>(-201) was performed at a substrate temperature 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 enhance nucleation, a nitridation step was performed for 5 min. During this time, we observed the evolution of the reflection high-energy electron diffraction (RHEED) pattern, transitioning from that of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>(-201) to GaN{0001}. After the nitridation step, AlN deposition under Al-rich conditions led to the appearance of a bright ring RHEED pattern, as an indication of polycrystalline growth without any preferential texture. The resultant samples exhibited a mirror-like surface with brownish coloration. AFM images of a 20-nm-thick AlN layer grown under these conditions show a root-mean-squared (rms) surface roughness around 3.0 nm. Further experiments were performed under N-rich conditions. In this case, the pattern evolves smoothly towards that of monocrystalline wurtzite AlN. After growth, the samples present mirror-like surface and they are optically transparent. AFM images show a flat morphology with 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  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>(-201) substrate. Transmission electron microscopy images of the interface show a sharp transition from the monoclinic  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> to wurtzite AlN lattices, with the presence of an intermediate wurtzite AlGa<sub>2</sub>N layer (thickness <1 nm). These results are promising for the fabrication of hybrid devices based on nitride/oxide heterostructures.