Structural characterization of GaN layers grown on graded-AlGaN/GaN/*c*-Al_2O_3 templates by HRXRD, GIXD, AFM and TEM

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Recently, a fundamentally new type of p-n junction have been successfully fabricated using compositionally graded $Al_xGa_{1-x}N$ films [1-2]. The doping enhancement occurs from grading the composition of $Al_xGa_{1-x}N$ alloys along the c-axis and thus grading the magnitude of the intrinsic polarization in the wurtzite crystal structure. Due to the ~2.4% lattice mismatch between AlN and GaN, tensile stress is induced in the $Al_xGa_{1-x}N$ film when growing on the GaN substrate. The increase of AlN molar fraction initiates the formation of misfit dislocations (MDs) and the crack networks in the graded $Al_xGa_{1-x}N$ films.

In this work, we investigate the deterioration mechanism of the graded $Al_xGa_{1-x}N$ thin films and their influence on the GaN cap layers, as a function of the AlN molar fraction and direction of the compositional gradient. The Al concentrations, strain evolution and structural quality in the graded $Al_xGa_{1-x}N$ films were determined by high-resolution x-ray diffraction (HRXRD). The grazing incidence x-ray diffraction (GIXD) was used to determine the in-plane strain and the structural quality of the GaN cap layers. The cross-sectional transmission electron microscopy (TEM) were applied to characterize the film structural qualities and the MDs behaviors. Atomic force microscopy (AFM) and optical microscopy were used to characterize the surface morphology of the samples.

It was observed that the cracks density on the GaN surface depends on the AlN molar fraction in the $Al_xGa_{1-x}N$ layers and the gradient direction. The highest cracks density was seen on the surface of sample with highest AlN molar fraction. This is accompanied with the decrease of the surface pits associated with the screw and mixed dislocations, which indicates on the cracks influence on the dislocation termination. For all samples, the cracks are overgrown at some points of their length which indicates that the cracks have formed during the growth. The full width at half maximum (FWHM) of HRXRD 0002 and GIXD $11\bar{2}0$ ω scans were correlated with the cracks and dislocations density on the samples surface.

1. J. Simon et al., Polarization-induced Hole Doping in Wide-Band-Gap Uniaxial Semiconductor Heterostructures. *Science*, 2010, 327, pp. 60-64.
2. A. Kuchuk. Nanoscale Electrostructural Characterization of Compositionally Graded $Al_xGa_{1-x}N$ Heterostructures on GaN/Sapphire (0001) Substrate. *ACS Appl. Mater. Interfaces*, 2015, 7 (41), pp 23320-23327.