The Role of Film Thickness on the Visible/UV and Infrared Optical Properties of GaN Films Grown By Hollow-Cathode Plasma-Assisted Atomic Layer Deposition

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In this study, we have studied and compared the optical properties of highly oriented (002) GaN films with different thicknesses, ranging from 5 to 100 nm deposited on Si, and quartz substrates via low-temperature hollow-cathode plasma-assisted atomic layer deposition (HC-PALD). Although the compressive stress is a result of lattice mismatch between GaN films and the substrates, it has been reported that the average strain in GaN thin films strongly correlates to the film thickness and usually changes from compressive to tensile with increasing thickness. In the present research, the evolution of the average strain, phonon position, and optical band gap energy in HCPA-ALD-grown GaN films have been analyzed. GaN thin films were prepared using a sequential injection of TEG and N₂/H₂ plasma within the self-limited growth regime, i.e., ALD window at 200°C. The grazing-incidence XRD scans of all GaN samples revealed that the films are crystalline with hexagonal wurtzite structure. Four main Bragg peaks corresponding to (002), (110), (103) reflections and a cumulative peak that encloses the (200), (112), and (201) reflections were observed. (002) and (103) diffraction signals become dominant at higher film thickness values. The films have been characterized from the mid-infrared to the ultraviolet spectral range by using spectroscopic ellipsometry in order to obtain the critical optical parameters including optical band edge and refractive index which helped us to understand the effect of film thickness on these parameters. The measurements indicate that the increasing trend of the refractive index reverses to decreasing behavior at ~60 nm. However, we have not observed a clear correlation between optical band gap and film thickness. The optical band edge values obtained from ellipsometry and optical transmission spectra are similar and the lowest bandgap value is ~3.55 eV. The optical band edge results suggested that bandgap widening is valid for all HCPA-ALD grown GaN samples. Phonon modes in GaN films were studied by employing infrared spectroscopic ellipsometry. The E₁(κ) and A₁(κ) phonon modes were identified for all four samples. All the phonon peaks related to GaN are considerably blue shifted with respect to their bulk values. This particular behavior is similar to the ones observed in GaN quantum dots. The E₁(κ) and A₁(κ) phonon modes are following comparable trend where the phonon peak positions shift towards lower wavenumbers for increasing thickness up to ~60 nm, while the phonon peak positions redshifted towards the bulk value for film thicknesses > 60 nm. The overall results suggested that GaN films with thicknesses above 60 nm have different behavior compared to the thinner GaN films.

Figure GIXRD patterns of HCPA-ALD GaN films grown on Si (100) (left). The infrared dielectric functions of the GaN films with different thickness. ε₁ and εᵢ correspond to the real and imaginary parts of the dielectric functions, respectively (right).