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Pseudomophic growth of GaN on AlN single crystal and template substrates by NH_3-MBE

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Over the past two decades III-nitrides have proven to be a promising material system for high electron mobility transistors operating at high frequency / high power due to their physical properties such as wide band gap and high electron saturation velocity. The two-dimensional electron gas needed for such devices has been formed so far mostly in heterostructures by combining alloys such as AlGaN and InAlN with the binary compound GaN on Si, sapphire and SiC wafers. The large lattice and thermal expansion coefficient mismatch between III-nitrides and those substrates leads to many issues ranging from high dislocation density, cracking and buffer leakage to inefficient heat management.

The lack of native substrates in the past has restrained III-nitrides from reaching their full potential. Fortunately the development of high quality bulk single crystals of GaN and AlN has experienced a great deal of progress over the last few years. Now high quality AlN single crystal substrates (<100 arcsec FWHM rocking curve) have become commercially available with physical properties which promise to outperform other material groups used for power devices. AlN is an excellent thermal conductor (κ = 285 $WK^{-1}m^{-1}$) and electrical insulator (E_g = 6.2 eV) and is therefore ideal for high power devices. Furthermore the low dislocation density (<10^3 cm^{-2}) of such substrates makes them very attractive for the growth of pseudomorphic layers. These are almost free from dislocations leading to a reduction of parasitic gate leakage channels. Recently we have shown that the critical thickness for the onset of plastic relaxation of GaN on AlN templates (grown on sapphire) ranges from 16 to 3 monolayers (ML) when increasing the substrate temperature from 750 to 900 °C. Based on the phenomenological kinetic theory of strain relaxation proposed by Dodson and Tsao we expect the critical thickness to also depend on the pre-existing dislocation density.

In this study we investigate the growth of III-nitrides on *c*-plane single crystal AlN substrates by NH_3-MBE. As a first step we examined the homoepitaxy of AlN as a function of substrate temperature and clearly observed the growth mode transition from 2D nucleation to step-flow by the vanishing of RHEED intensity oscillations with increasing temperature. A smooth initial epitaxial layer can be achieved by growing AlN at a high temperature (1150 °C) in the step-flow regime. Due to the low dislocation density (<10^3 cm^{-2}) of the substrates we were interested in following the evolution of the strain relaxation and the critical thickness of GaN layers grown on AlN by monitoring *in situ* the variation of the in-plane lattice constant given by the RHEED streak spacing. We observe an enhancement of the critical thickness by at least a factor of 2 compared to layers grown on AlN/sapphire templates (high dislocation density ≈ 10^9 cm^{-2}) which demonstrates the crucial role of pre-existing dislocations on the mechanism governing strain relaxation in III-nitrides. The enhanced critical thickness allows pseudomorphic growth of thicker layers promoting novel heterostructures of high quality which are expected to improve the efficiency of future devices.