TEM Analysis of Defects in AlGaN Heterostructures Grown on c-Al₂O₃ by Plasma Assisted Molecular Beam Epitaxy

Sergei Rouvimov^{1,2}, V. N. Jmerik³, D.V. Nechaev³, and S.V. Ivanov³

^{1.} Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana 46556, USA
^{2.} Notre Dame Integrated Imaging Facility, University of Notre Dame, Notre Dame, Indiana 46556, USA

³ A. F. Ioffe Physical-Technical Institute, 194021, 26 Politekhnicheskaya str., St.-Petersburg, Russia

This paper addresses the defect formation in AlGaN-based heterostructures with high Al-content (x>0.4) grown by plasma assisted molecular beam epitaxy (PA MBE). The growth of AlGaN epitaxial layers with reduced defect density is a challenging technological task that requires understanding of defect generation and propagation. Low defect density in AlGaN-based heterostructures is critical for fabrication of high efficiency optoelectronics devices such as UV- emitters with wavelength below 300 nm. The reduction of threading dislocation (TDs) densities allows for better control of the carrier's transport and residual stress in the optically-pumped UV-laser structures grown over standard c-sapphire substrates by using PA MBE. Here we review defect generation in AlGaN heterostructures to understand the mechanisms of their formation especially at initial growth stages.

The samples were analyzed by TEM using both high resolution TEM (HRTEM) and High Angle Annual Dark Field (HAADF) scanning TEM (STEM) modes at FEI Titan 80-300 electron microscope. The microscope was operated at 300 keV and equipped with an Oxford Inca EDX detector. TEM cross-sectional samples were prepared by Focus Ion Beam (FIB) using FEI Helios SEM/FIB dual beam equipment.

It was demonstrated that migration-enhanced epitaxy (MEE) of the AlN buffer layer and 3D growth of ultra-thin GaN interlayers in AlN layers result in substantial reduction of dislocation density in AlGaN-based heterostructures. Figure 1 shows typical Bright Field (BF) TEM images of AlN layers demonstrating that the threading dislocations are mainly of edge type (Fig. 1a). The enlarged BF TEM image in Fig. 1c shows the formation of voids at AlN-sapphire interface. One can speculate that the lateral overgrowth of separated AlN islands may reduce strain at the initial growth stage while increasing the size of the islands, and, as a result, leading to subsequent reduction of TD generation at epi-substrate interface.

The other approach for the reduction of the dislocation density includes ultra-thin GaN interlayers (Fig. 1) in AlN layers that lead to abrupt stress at AlN/GaN interface during the growth and, as a result, to dislocation bending into the interface with their further annihilation ("blocking" effect). This approach was shown to result in the reduction of dislocation density down to 10^{8} - 10^{9} cm⁻² in the top (active) part of (2-3)-µm-thick heterostructures. In addition, the precise control of the stress in AlGaN layers was achieved by a digital alloying technique and with optimization of growth parameters. HAADF STEM imaging (Fig. 3) evidences the presence of aperiodic superlattices (alternating Al- and Ga-rich AlGaN monolayers) formed in AlGaN cladding and waveguide layers grown under strong metal-enriched stoichimetrical conditions. Analysis of HAADF STEM images of AlGaN waveguide layers (Fig. 3) revealed the presence of 1-ML-thick Ga-enriched disks distributed in the nominally 2-nm-thick Al_xGa_{1-x}N/Al_yGa_{1-y}N(x=0.5-0.7, y-x=0.1) SQW-structures in accordance with the growth cycle sequences in the sub-monolayer digital alloying technique. The mechanisms of defect generation in such hetero-epitaxial structures are discussed.

References:

[1] S. V. Ivanov, D. V. Nechaev, A. A. Sitnikova, V.V. Ratnikov, M.A. Yagovkina, N. V. Rzheutskii, E. V. Lutsenko, and V. N. Jmerik, *Semicond.Sci.Technol.* **29**, 084008 (2014).



Figure 1 BF TEM images (a, b) of AlN layers with GaN inserts taken at two perpendicular **g** vectors to compare the dislocation density with edge (a) and screw (b) components. Image (c) is enlarged BF TEM image of MEE AlN buffer layer showing voids at the AlN-sapphire interface.







Figure 3. HAADF STEM images of $Al_{0.6}Ga0.4N$ waveguide layer with 2-nm-thick SQW showing formation of spontaneous super lattice in the waveguide layer.