**Molecular Beam Epitaxy Of Gan On Lattice-Matched $Zrb_2$ Substrates Using Low-Temperature Gan And Aln Nucleation Layers**


Rob Armitage, Jun Suda, and Tsunenobu Kimoto

Department of Electronics Science and Engineering
Kyoto University
Katsura, Nishikyo-ku, Kyoto 615-8510, Japan


Zirconium diboride is an intriguing substrate for (Al)GaN heteroepitaxy due to its closely matched in-plane lattice constant and thermal expansion coefficient. For some applications (e.g. laser diodes, power switches) the high electrical and thermal conductivities of $ZrB_2$ are additional advantages. However, heteroepitaxy of GaN on $ZrB_2$ is challenging due to poor wetting at typical growth temperatures (e.g. 700°C). In the present work we study low-temperature GaN (LT-GaN) and AlN nucleation layers for growth of high-temperature GaN on $ZrB_2$ by rf-MBE.

Low-temperature GaN nucleation layers on $ZrB_2$ result in nitrogen polarity for all conditions investigated. The GaN main layer properties are highly sensitive to the Ga/N ratio of the LT-GaN. LT-GaN nucleation in slightly N-rich conditions yields high-temperature GaN with a very smooth morphology. Atomic steps are observed across the length of 10 um AFM scans. Despite this the x-ray omega scans for such layers are rather poor: 14 arcmin for the (0002) and 19 arcmin for the (1-104) peak. When LT-GaN nucleation is performed in slightly Ga-rich conditions, the main layer x-ray characteristics significantly improve (7 and 14 min, respectively), but the morphology shows a sub-grain structure without clear steps (Fig. 2). This difference may be related to the grain structure of the LT-GaN nucleation layer.

AlN nucleation layers lead to either Ga-polar or N-polar GaN main layers depending on the AlN thickness and deposition temperature. For nucleation at 550°C an AlN layer as thin as 1-2 nm can yield Ga-polarity, while for nucleation at 700°C a thicker AlN layer (>5 nm) is necessary to ensure Ga-polarity. Ga-polar GaN layers on $ZrB_2$ exhibit the spiral hillock morphology. The AlN nucleation process has not been optimized yet, but the x-ray FWHM for preliminary Ga-polar layers are 17 and 24 arcmin for the (0002) and (1-104) peaks, respectively.

The low-temperature photoluminescence spectrum of GaN grown using an LT-GaN nucleation layer on $ZrB_2$ with optimized main layer growth conditions is shown in Fig. 3. The FWHM of the $D_0X$ peak is 10 meV at 18 K and the peak intensity ratio between 18 K and room temperature is about 100. The $D_0X$ peak appears at 3.743 eV indicating the crystal is almost strain free, consistent with the good thermal and lattice match of $ZrB_2$.

Additional experiments are now underway using exactly lattice-matched $Al_{0.24}Ga_{0.76}N$ nucleation layers. It is expected that coalescence of strain-free nuclei (as opposed to strained GaN or AlN nuclei) will lead to reduced tilt and twist misorientation and thus reduce the defect density in the main GaN epilayer.

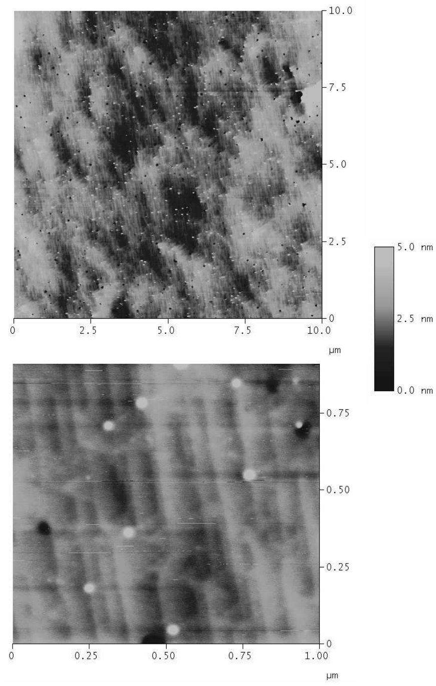


Fig. 1. **Top:** 10 um AFM scan of a 0.5 um N-polar epilayer using a LT-GaN nucleation layer grown in slightly N-rich nucleation conditions. **Bottom:** Magnification of the above image clearly showing atomic steps. Scale 5 nm, rms <0.5 nm over 10 um.

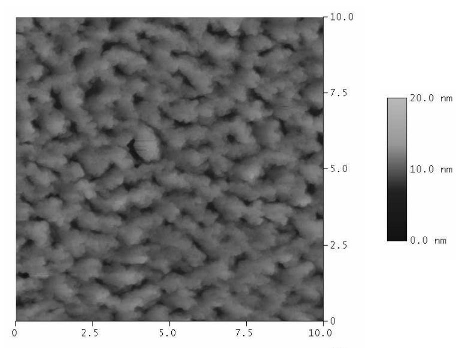


Fig. 2. 10 um AFM scan of a 0.5 um thick N-polar GaN epilayer using a LT-GaN nucleation layer grown in slightly Ga-rich nucleation conditions. Scale 20 nm.

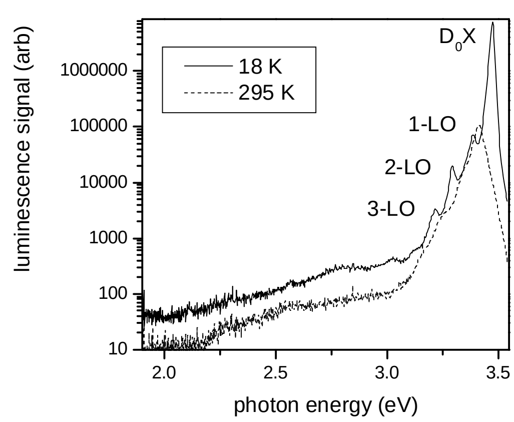


Fig. 3. Photoluminescence spectra at 18K and 295K for the sample of Fig. 2. Phonon replicas of the donor-bound exciton ($D_0X$) peak are denoted "–LO."