

Thursday Morning, October 21, 2010

Electronic Materials and Processing

Room: Dona Ana - Session EM+SS-ThM

Nitride Surfaces and Interfaces

Moderator: Engel-Herbert, Penn State University

8:00am **EM+SS-ThM1 Recent Advances in the MOCVD Growth of III-N Light Emitting Diodes**, *R.D. Dupuis, J.-H. Ryou, H.-J. Kim, J. Liu, Z.M. Lochner, J. Kim, S. Choi, S.-S. Kim*, Georgia Institute of Technology
INVITED

Group III-nitride-based green light-emitting diodes (LEDs) are increasingly used in applications for full-color displays, back-lighting, and color-mixing-based general illumination lighting systems. Recently, the potential for III-N LEDs to replace all forms of conventional lighting sources has been discussed and advanced white-light LEDs have entered the market place for general consumer use. However, significant fundamental and technical challenges remain for III-N LEDs to achieve their full potential, such as the improvement of the peak internal quantum efficiency (IQE) and the minimization of the efficiency droop with increasing injection current density. For full-color lighting based upon III-N RGB LEDs, other impediments remain. The peak IQE of green LEDs are significantly lower than shorter-wavelength InAlGaP-based blue and longer-wavelength InAlGaP-based red LEDs, a feature referred to as a "green gap". In addition, the efficiency of green LEDs at high drive currents decreases with increasing injection current more significantly than in blue LEDs. In this paper, we will review some of the recent work and advances in the area of improving the high-current-density performance of III-N LEDs.

8:40am **EM+SS-ThM3 Microstructural Comparison of InGaN/GaN Multi Quantum Wells Grown on SiC and GaN Substrates**, *F. Liu, L. Huang*, Carnegie Mellon University, *E.A. Preble, T. Paskova, K. Evans*, Kyma Technologies, Inc., *R.F. Davis, L.M. Porter*, Carnegie Mellon University

Light emitting diodes (LED) with InGaN/GaN multi-quantum wells (MQW) as the active region are now being widely investigated for blue and green light sources. However, InGaN/GaN MQWs grown on sapphire or SiC substrates commonly contain V-shaped defects with densities as high as 10^9 cm^{-2} . These V-defects, which are believed to degrade the internal quantum efficiency of the LED, are remarkably reduced via growth on GaN substrates. In this study, we present a detailed microstructural comparison between $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ (3nm)/GaN (8nm) MQWs grown on AlGaP/SiC (0001) and GaN (0001) substrates via metalorganic chemical vapor deposition at 790°C. The composition was determined by analyses of x-ray diffraction (XRD) and photoluminescence measurements. The microstructure was characterized using a variety of techniques, including transmission electron microscopy (TEM), scanning electron microscopy (SEM), electron channeling contrast imaging (ECCI), and photoelectrochemical (PEC) etching. SEM images revealed that the V-defect density decreased from $1 \times 10^{10} \text{ cm}^{-2}$ to $7 \times 10^6 \text{ cm}^{-2}$ in MQWs grown on SiC and GaN substrates, respectively. Cross-sectional TEM images on MQWs grown on SiC substrates indicated that V-defects invariably originated from threading dislocations. To test this hypothesis, we investigated the threading dislocation densities prior to the growth of the MQWs (i.e., in (300-500 nm) GaN films grown on SiC and GaN substrates) via PEC etching and ECCI. The dislocation densities observed in these samples ($\sim 6 \times 10^9 \text{ cm}^{-2}$ on SiC; $\sim 4 \times 10^6 \text{ cm}^{-2}$ on GaN) are close to the respective densities of V-defects observed in samples after growth of the MQWs. These results from multiple techniques provide convincing evidence that the dislocation densities in the GaN layer above the substrate determine the densities of V-defects in the MQW. The introduction of dislocations directly from GaN substrates into the homoepitaxial layers is also under investigation using the techniques described herein.

9:00am **EM+SS-ThM4 Switching GaN Polarity on Homoepitaxial Substrates**, *J.K. Hite, M.E. Twigg, M.A. Mastro, F.J. Kub, C.R. Eddy, Jr.*, Naval Research Laboratory

Gallium nitride (GaN), a highly advantageous material for both optical and electronic devices, can be grown in the (+/-) c-direction of its lattice with two different polar faces, nitrogen- (N-) or gallium- (Ga-) polar. The face or polar orientation of the material establishes many quite varied properties of the material, from chemical reactivity to dopant incorporation to spontaneous and piezoelectric-induced electric field directions in the crystal. Control of the polarization fields and, thus, polarization induced doping is the basis of Ga-polar and N-polar GaN-based high electron mobility transistor operation. On heterogeneous substrates, such as silicon

carbide (SiC) and sapphire (Al_2O_3), the growth conditions, doping levels, and buffer or nucleation layer properties are used to control the polarity of resulting GaN epilayers. Further, in the case of heavily doped p-type layers, spontaneous polarity inversion has been demonstrated even on GaN epilayers, switching from Ga-polar to N-polar in the doped layer.¹ However, this approach leads to uncontrolled inversion domain boundaries and often results in dopant clustering² in the film, impacting film quality and resultant device performance.

In contrast, this new approach enables the controlled formation of Ga-polar GaN from a N-polar crystal. Instead of using concentrated doping, the polarity switch in this case hinges on both surface treatment and the addition of an optimized polarity inversion layer. Initial material characterization verified that the film was without N-polar inclusions or inversion domain boundaries. Chemical etching of the material in 4M KOH under slightly elevated temperatures (40°C) for 10-40 minutes as well as convergent beam electron diffraction³ are employed to verify the polarity of the films. The structural quality of the films is ascertained with transmission electron microscopy and x-ray diffraction. In addition, the dislocation density and grain size are determined through the use of electron channeling contrast imaging.⁴ While lateral polarity heterostructures have been of interest due to their unique electrical and structural properties,⁵ this method offers the promise of engineering both lateral and vertical polarity heterostructures and the potential of novel variable polarity-based devices.

¹V. Ramachandran et al., Appl. Phys. Lett. **75**, 808, 1999.

²M. Hansen et al., Appl. Phys. Lett. **80**, 2469, 2002.

³F.A. Ponce et al., Appl. Phys. Lett. **69**, 337, 1996.

⁴Y.N. Picard et al., Appl. Phys. Lett. **91**, 094106, 2007.

⁵M. Stutzmann et al., Phys. Status Solidi b **288**, 505, 2001.

9:20am **EM+SS-ThM5 Studies of InGaN Growth Morphology and Its Relationship to Multiple Quantum Well Luminescence**, *D. Koleske, S.R. Lee, M.H. Crawford, M.E. Coltrin, J.M. Kempisty, K.C. Cross*, Sandia National Laboratories

It has been suggested that InGaN quantum well (QW) thickness fluctuations, acting in conjunction with piezoelectric fields, are sufficient to cause exciton localization and reduce non-radiative recombination at dislocations [1]. Consequently, the study of InGaN step morphology and the control of InGaN/GaN interfaces may be crucial for understanding and improving blue and green LED quantum efficiency. To this end, a variety of InGaN QW and thin film structures have been grown to determine how the surface roughens when GaN is alloyed with InN. Statistical analysis of the step-height distributions from AFM images shows that the nominally single-layer step heights transition to multiple-layer step heights as InGaN is grown on GaN. Further analysis of the surface-roughness power spectral density suggests that the main smoothing mechanism changes from an evaporation/recondensation mechanism to a surface diffusion mechanism as the growth temperature is lowered to incorporate indium into GaN. Exploiting these two smoothing mechanisms allows the construction of otherwise identical MQW structures with smoother or rougher InGaN QW interfaces. Initial studies of the correlations between QW interface roughness and luminescence intensity suggest that some degree of InGaN QW roughness leads to higher luminescence efficiency, lending credibility to theories that propose a structural-based enhancement of exciton localization. [1] D. M. Graham, *et al.*, J. Appl. Phys. 97 103508 (2005).

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9:40am **EM+SS-ThM6 High-Quality, Large-Area, and Free-Standing GaN Epilayer Growth and Liftoff using Self-Assembled Interlayer of Silica Microspheres**, *Q. Li, G.T. Wang*, Sandia National Laboratories

We demonstrate that self-assembled monolayers of silica microspheres can be used as inexpensive, selective growth masks for both significant threading dislocation density reduction and laser-free lift-off of GaN epilayers and devices. Silica microspheres self-assemble into close-packed monolayers on the surface of an initial GaN epilayer on sapphire using a Langmuir-Blodgett method. In a subsequent GaN regrowth, the silica microspheres effectively terminate the propagation of threading dislocations. As a result, the threading dislocation density, measured by large area AFM and CL scans, is reduced from $3.3 \times 10^9 \text{ cm}^{-2}$ to $4.0 \times 10^7 \text{ cm}^{-2}$. This nearly two orders of magnitude reduction is attributed to a dislocation blocking and bending by the unique interface between GaN and silica microspheres. The sequential wet etching of the samples in HF

solution removes the silica microspheres sandwiched between the GaN epilayers and the growth template. Further wet etching of the samples in KOH solution successfully detaches the GaN epilayers from the growth templates. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

10:40am **EM+SS-ThM9 GaN(0001) Surface at Various Conditions: Fundamental Properties and Basic Dynamic Processes - Ab Initio Study, S.K. Krukowski**, Polish Academy of Sciences, Poland **INVITED**

Due to its polar nature, gallium nitride, GaN properties strongly depend on its orientation. Therefore various GaN surfaces have different physical properties, which is related to their different atomic structure and also to the different electric fields in the subsurface layers. A new developed procedure allows to simulate these fields exactly, in a controlled fashion, within the slab model, by modification of the termination of the opposite side of the slab. These techniques will be discussed using bare Ga-terminated GaN(0001) surface as a working example. It will be shown that the field causes shift of the energy of the surface and band states, which is known as Surface States Stark Effect (SSSE). This approach will be employed also in the discussion of the hydrogen covered GaN(0001) surface. Both equilibrium properties and dynamic processes will be investigated with the account of the role of electric field, or equivalently doping in the bulk semiconductor, in shaping of the surface electronic and energetic properties. Equilibrium properties such as hydrogen adsorption sites and energy, and also the thermodynamic and energetic stability will be discussed for various coverage. It will be shown that adsorption of molecular hydrogen on bare GaN(0001) surface leads to its dissociation and location of H atoms in the sites, above the Ga surface atoms. The interaction with adsorbed species leads to strong relaxation of the surface with Ga atoms moving upwards towards H adatoms. Generally, the hydrogen adatoms are strongly confined at the GaN(0001) surface, having their energy 1 eV below that in the GaN bulk. Thus the hydrogen coverage of GaN (0001) surface is stable, and its removal is extremely difficult. The energy of H - induced surface states strongly depend on the doping in the bulk: in p-type GaN the state is close to valence band maximum, but for n-type it is located 2 eV lower. The determined dynamic properties include the adsorption paths showing that the adsorption of molecular hydrogen depends on the coverage: for small coverage, molecular hydrogen is chemically adsorbed at the surface while for 1ML H-coverage it encounters significant energy barriers, drastically lowering the probability of this process. Adsorption of atomic hydrogen does not depend on the coverage, leading at some instances to creation of H₂ admolecules which subsequently could be desorbed from the surface.

The research was partially supported by the European Union within European Regional Development Fund, through grant Innovative Economy (POIG.01.01.02-00-008/08).

11:20am **EM+SS-ThM11 Surface Photovoltage Behavior for p-type vs. n-type GaN, A.A. Baski, M. Foussekis, M.A. Reshchikov**, Virginia Commonwealth

Devices based on wide-bandgap GaN are successfully being used today, but a better understanding of surface effects such as band bending could further improve their performance. Many results have been reported on the upward surface band bending for n-type GaN, but fewer exist on the downward band bending for p-type GaN. Surface photovoltage (SPV) measurements using a Kelvin probe can directly measure the change in surface potential during UV illumination, and thereby indirectly measure the resulting decrease in band bending. We have studied steady-state and transient SPV for band-to-band (365 nm) illumination on a variety of p-type (Mg-doped) and n-type (Si-doped) GaN samples grown by hydride vapor phase epitaxy and metal organic chemical vapor deposition.

For n-type and p-type GaN samples, short (5 s) UV exposures generate an SPV magnitude of about 0.5 eV in both air and vacuum environments. The sign of the SPV signal is positive for n-type GaN and negative for p-type GaN, corresponding to a positive or negative change in surface potential, respectively. This fast component of the SPV corresponds to the accumulation of photo-generated holes (n-type) or electrons (p-type) at the semiconductor/oxide interface and leads to a corresponding decrease in band bending. As expected, this "internal" mechanism does not appear to depend on the sample environment. After ceasing illumination, decay of the SPV in dark and under all environments is slow with a logarithmic time dependence.

It is during longer UV exposures that the SPV behavior becomes noticeably different for n- vs. p-type samples. For n-type GaN, a long UV exposure (1 h) typically causes the SPV to decrease to 0.35 eV in air, but to increase to 0.6 eV in vacuum. This SPV behavior is consistent with the photo-induced adsorption of negatively charged oxygen species in air and their desorption in vacuum. In contrast, long UV exposure for some p-type samples has caused the SPV to reach a surprisingly large value of -1.1 eV in air, but to

not change significantly in vacuum. The more negative SPV in air again indicates the adsorption of negative surface species, but the rather large change over extended illumination is not expected, particularly given that a comparable opposite change does not occur in vacuum (as for n-type). Therefore, the charging of the surface layer on p-type GaN and how it affects band bending is still under investigation. We have developed a phenomenological model that is able to distinguish contributions from internal (fast) and external (slow) mechanisms in SPV transients, and have demonstrated that the native oxide layer can play a significant role.

11:40am **EM+SS-ThM12 Investigation of the Structure of GaN(0001) Pseudo-1x1 Structure at Low Temperature, A.R. Smith, T. Chen, K. Wang, Y. Liu**, Ohio University Nanoscale and Quantum Phenomena Institute

The wurtzite GaN(0001) surface has previously been determined to be in a pseudo-1x1 structure which includes approximately 2 monolayers (ML's) of Ga sitting atop the last GaN bilayer [1]. This metallic structure, commonly observed, was initially determined using a combination of reflection high energy electron diffraction (RHEED), Auger electron spectroscopy, and scanning tunneling microscopy (STM). In addition, there has been theoretical work performed for this surface. [2,3] In RHEED, the main observation is the appearance of satellite streaks located at 1/6th (or 1/12th) of the primary streak spacing outside of the primary streaks. It was initially modeled as a bi-axially contracted Ga bi-layer, contracted by approximately 16% relative to the GaN bulk. Theoretical calculations found only the top Ga ML to be contracted bi-axially. More recent theory work by Rinehimer et al. suggest that instead it is uniaxially contracted but having a similar structure. [3]

We investigate the pseudo-1x1 structure experimentally using a new growth and analysis system consisting of a molecular beam epitaxy (MBE) chamber for preparation of the surface and a RHEED system to monitor it. The sample growth stage also has the feature of allowing cooling to cryogenic temperatures as well as heating. The pseudo-1x1 structure is prepared by MBE growth on MOCVD-grown GaN substrates. Following this, the sample is cooled down, and the diffraction pattern is monitored. At low temperature, we observe the onset of new diffraction streaks located at approximately 5/12 and 7/12 of the primary streak positions, as well as disappearance of the pseudo-1x1 satellite streaks.

Models for the low-temperature GaN(0001) structure are currently being formulated which may give new insights into the structure of the pseudo-1x1, based on this new low-temperature RHEED data. As one model currently under consideration, a uniaxial, aperiodic superstructure is proposed in which the top Ga layer freezes into a coherent layer but with the resultant extra Ga atoms being displaced vertically. To further probe this model, low-temperature STM experiments are currently being planned, to be conducted in an adjacent in-situ STM system. This work is supported by the National Science Foundation (Grant No. 0730257) and by a grant from Ohio University.

[1] A. R. Smith, R. M. Feenstra, D. W. Greve, M.-S. Shih, M. Skowronski, J. Neugebauer, and J. E. Northrup, *J. Vac. Sci. Technol. B* **16** (4), 2242 (1998).

[2] J. E. Northrup, J. Neugebauer, R. M. Feenstra, A. R. Smith, *Phys. Rev. B* **61**, 9932 (2000).

[3] J.A. Rinehimer, M. Widom, J.E. Northrup, and R.M. Feenstra, *Phys. Stat. Sol. (b)* **245**(5), 920 (2008).

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