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**Theoretical Study of Point Defects in GaN and AlN: Lattice Relaxations and Pressure Effects**

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Native defects and some common dopants (Mg, Zn, and C) in cubic GaN and AlN are examined by means of *ab initio* theoretical calculations using two methods: i) the Green's function technique based on the linear muffin-tin orbital method in the atomic-spheres approximation; ii) a supercell approach in connection with the full-potential linear muffin-tin-orbital method. We apply the first method to look mainly at the energetic positions of the defect and impurity states in different charge states and their dependence on hydrostatic pressure. The second method allows us to study lattice relaxations. Whereas small relaxations are found near vacancies and substitutional Mg and Zn, the calculations predict large atomic displacements around antisite defects and the substitutional carbon impurity on the cation site.

**Order No. NS002-018** 

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**A Perspective on the GaN Injection Laser**

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This short paper is a brief review of the problems to be overcome for making an injection laser using a new semiconductor that promises to revolutionize the information storage industry.

**Order No. NS002-019** 

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**Evidence of 2D-3D Transition During the First Stages of GaN Growth on AlN**

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In order to identify the strain relaxation mechanism, molecular beam epitaxy of wurtzite GaN on AlN was monitored *in situ* using reflection high energy electron diffraction (RHEED). In the substrate temperature range between 620°C and 720°C, a Stransky-Krastanov (SK) transition was evidenced, resulting in a 2D-3D transition after completion of 2 monolayers, with subsequent coalescence of 3D islands, eventually resulting in a smooth surface. Quantitative analysis of the RHEED pattern allowed us to determine that island formation is associated with elastic relaxation. After island coalescence, a progressive plastic relaxation is observed. The size and density of 3D islands was varied as a function of the growth parameters. AFM experiments revealed that the size of the GaN islands, about 8 nm large and 2 nm high, was small enough to expect quantum effects. It was found that capping of the islands by AlN resulted in a smooth surface after deposition of a few monolayers allowing us to grow a "superlattice" of islands by periodically repeating the process.

**Order No. NS002-020** 

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**Optical Nonlinearities of Gallium Nitride**

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Luminescence, induced absorption, and degenerate four-wave mixing experiments are performed on GaN epilayers grown on a sapphire substrate by MOCVD.

We measure the nonlinear behavior of the luminescence spectra near the excitonic resonance, by using an excitation at 4.026 eV from an excimer laser. At low intensities of excitation, spectra show a saturation of the $I_2$ line due to the finite donor density in the sample. Higher intensities of excitation induce collision processes between photo-created quasi-particles.

Using a dye laser as a pump beam, we measure the induced variation of absorption of a probe beam as a function of the intensity and of the wavelength of the excitation. With increasing intensities of the pump beam, transmission spectra show a red-shift of the absorption edge and of the excitonic resonance.

Pulsed degenerate four-wave mixing experiments were performed using the third harmonic of a picosecond Nd-YAG laser at 3.492 eV. A characteristic time constant of 16 ps has been measured, which is independent of the temperature, spacing of the interference fringe and of the intensity of the pump beams.

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**AlGaN-Based Bragg Reflectors**

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We have studied the dependence of the absorption edge and the refrac-

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tive index of wurtzite $Al_xGa_{1-x}N$ films on composition using transmission, ellipsometry, and photothermal deflection spectroscopy. The Al molar fraction of the $Al_xGa_{1-x}N$ films grown by plasma-induced molecular beam epitaxy was varied through the entire range of composition ($0 \leq x \leq 1$). We determined the absorption edges of $Al_xGa_{1-x}N$ films and a bowing parameter of 1.3 ± 0.2 eV. The refractive index below the bandgap was deduced from the interference fringes, the dielectric function between 2.5 and 25 eV from ellipsometry measurements. The measured absorption coefficients and refractive indices were used to calculate the design and reflectivity of AlGaN-based Bragg reflectors working in the blue and near-ultraviolet spectral region.

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**XPS Study of Au/GaN and Pt/GaN Contacts**

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Au/GaN and Pt/GaN contacts have been studied with XPS. According to XPS depth profiling, the N signal is weak in the region below the metal contact and the Pt or Au signal decreases much more slowly than expected for a sharp interface. Next, we have performed *in situ* studies of the formation of Au contacts on GaN. In contrast to the results from depth profiling, we observe 2D growth and little or no chemical interaction between Au and GaN. This suggests that conventional calculations of sputtering yields and ion-beam-induced mixing cannot be applied to the analysis of noble metal/GaN depth profiles. Heating during or after Au deposition results in strong clustering, observed by both XPS and AFM. The Schottky barrier height measured by XPS is 1.15 eV.

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http://nsr.mij.mrs.org/2/24/

**Transient Four Wave Mixing Experiments on GaN**

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We present four wave mixing experiments on GaN. We find an intrinsic homogeneous broadening of the A-exciton of 1.67 meV. A pronounced beating with a period of 0.52 ps is observed at excitation energies between the A- and the B-exciton and corresponds to an energy splitting of 7.98 meV of A- and B-exciton.

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**Properties of the Biexciton and the Electron-Hole-Plasma in Highly Excited GaN**

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High-excitation processes like biexciton decay and recombination of an electron-hole-plasma are discussed as efficient mechanisms for lasing in blue laser diodes. Therefore, the investigation of these processes is of fundamental importance to the understanding of the properties of GaN as a basic material for optoelectronical applications. We report on comprehensive photoluminescence and gain measurements of highly excited GaN epilayers grown by metal-organic chemical vapor deposition (MOCVD) over a wide range of excitation densities and temperatures. For low temperatures the decay of biexcitons and the electron-hole-plasma dominate the spontaneous-emission and gain spectra. A spectral analysis of the lineshape of these emissions is performed and the properties of the biexciton and the electron-hole-plasma in GaN will be disscused in comparison to other wide-gap materials. At increased temperatures up to 300 K exciton-exciton-scattering and band-to-band recombination are the most efficient processes in the gain spectra beside the electron-hole-plasma.

**Order No. NS002-025** 

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**Fundamentals, Material Properties and Device Performances in GaN MBE Using On-Surface Cracking of Ammonia**

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Ammonia is investigated as nitrogen precursor for molecular beam epita of group III-nitrides. With the particular on-surface cracking approach, N is dissociated directly on the growing surface. By this technique, molec beam epitaxy becomes a serious competitor to metal organic vapor p epitaxy. Thermodynamic calculations as well as experimental results re insights into the growth mechanisms and its differences to the conventi plasma approach. With this knowledge, homoepitaxially GaN can be gro with record linewidths of 0.5 meV in photoluminescence (4 K). GaN laye on *c*-plane sapphire also reveal reasonable material properties (photolum nescence linewidth 5 meV, $n \approx 10^{17}$ cm$^{-3}$, $\mu \approx 220$ cm$^2$/Vs). Beside Ga growth, *p*- and *n*-doping of GaN as well as the growth of ternary nitrides are discussed. Using the presented ammonia approach uv-LEDs emitting at 370 nm with linewidths as narrow as 12 nm have been achieved.

**Order No. NS002-026** 

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**MOVPE Growth and Structural Characterization of $Al_xGa_{1-x}$**

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The ternary alloy GaAlN has been grown by low pressure MOVPE (76 Torr) using triethylgallium, trimetylaluminum, and ammonia as precursors. The alloy layers were grown on (0001) sapphire substrates using a low temperature AlN buffer. All layers were deposited at a growth temperature of 980°C. Only the aluminum/gallium ratio in the gas phase was changed, keeping the total group III molar flow rate and V/III molar ratio constant.

The aluminum incorporation versus gas phase composition was determined experimentally, using energy dispersive analysis of x-rays (EDAX), and x-ray diffraction. We propose a model, taking into account kinetically limited mass transport of group III species in the gas phase, which describes well the data.

The structural quality of the layers was investigated using x-ray diffraction and TEM experiments.

A degradation of the materials quality is observed with increasing Al content. In this case, growth originate on the buffer grains facets resulting in a "two directional" growth. This phenomenon, being markedly enhanced when increasing the Al content will be detailed in this paper.

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**Yellow Luminescence in Mg-Doped GaN**

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Optical thresholds, that correspond to a level located at 1 eV above the valence band, are observed by photocapacitance techniques in *n*-type Mg-doped GaN. In undoped GaN, this level has been previously related to the yellow emission detected by photoluminescence. In Mg-doped GaN, this yellow luminescence is only observed for excitation energies below the Mg-related band (2.9 – 3 eV). This result evidences that Mg-doping may reduce but not avoid the formation of the yellow band related defects in *n*-type and semiinsulating Mg-doped samples. The fact that the yellow luminescence is not observed for excitation energies above the bandgap may be justified by



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a higher efficiency of the Mg-related recombination path.

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**Properties of InGaN Deposited on Glass at Low Temperature**

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We have investigated the properties of InGaN grown at low temperature h glass substrates by a plasma enhanced MBE process. The goal of this ıdy was to evaluate the potential of InGaN as an oxide-free, transparent ductor material which could be deposited at or slightly above room temature with minimal interaction or damage to the underlying material. $Ga_{1-x}N$ films deposited on glass, even without substrate heating, are high-crystalline, but the crystallinity as measured by x-ray degrades at $x < 0.5$. e microstructure observed by TEM of InGaN films deposited on unheated ubstrates is highly columnar, with typical column widths of ~10 nm. The ptical absorption spectra of InGaN/glass have a distinct absorption edge at he bandgap, but also high background absorption in the bandgap. $In_xGa_{1-x}N$ grown on glass ($x > 0.5$) is conductive due to its high electron concentration. InN electron Hall mobilities > 20 cm²/Vs when grown at 400°C, and ~ 7 cm²/Vs on unheated substrates were obtained. The addition of GaN degraded the electrical properties of the films to a greater extent than it improved the transparency. As a result, the best transparent conductor films were pure InN which, when deposited at 400°C, were half as transparent in the green as an indium tin oxide film having the same sheet resistance.

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**Epitaxial Growth and Orientation of GaN on (100) γ-$LiAlO_2$**

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The (100) face of γ-$LiAlO_2$ has attracted attention as a possible substrate for GaN epitaxial growth. This is partly because this face has an excellent lattice and structural match to (1$\bar{1}$00) GaN. This orientation would have a misfit of only -1.4% along the **c**-direction and -0.1% along the **b**-direction of $LiAlO_2$. We find that in practice this orientation relationship does not occur; instead, (0001) oriented GaN grows with a small tilt (0.6° towards the **c**-direction) between the film and substrate. Although the misfit along the substrate **b** direction is large (-6.3%) for this orientation, the tilt perfectly accommodates the -1.4% misfit in the **c** direction. We present characterization of these films by RHEED, x-ray diffraction, and TEM. We propose that the tilt is driven by a reduction of interface energy which occurs in polar, incoherent interfaces.

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**Comparison of Luminescence and Physical Morphologies of GaN Epilayers**

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In this paper we examine a series of four GaN epilayers grown by MOVPE on sapphire substrates with different AlN buffer layer thicknesses. We examine the effect of the buffer layer thickness on the physical and optical properties of the samples via optical microscopy, cathodoluminescence imaging, and photoluminescence and cathodoluminescence spectroscopy. While the morphological and optical properties of all the films (excepting that with the thinnest buffer layer of 30 nm) are good, i.e., the films are smooth and the luminescence is dominated by excitonic luminescence, a number of circular island like features are observed in all the films whose density decrease with increasing buffer layer thickness. A large circular island present on the sample with the thinnest buffer layer and surrounded by cracks in the <11$\bar{2}$0> directions, displays some interesting acceptor related luminescence.

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**Exciton Dynamics in Thick GaN MOVPE Epilayers Deposited on Sapphire**

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Time-resolved photoluminescence spectra have been recorded on three GaN epitaxial layers of thickness 2.5 μm, 7 μm and 16 μm, at various temperatures ranging from 8 K to 300 K. The layers were deposited by MOVPE on (0001) sapphire substrates with standard AlN buffer layers. To achieve good homogeneities, the growth was *in situ* monitored by laser reflectometry. All GaN layers showed sharp excitonic peaks in cw PL and three excitonic contributions were seen by reflectivity. The recombination dynamics of excitons depends strongly upon the layer thickness. For the thinnest layer, exponential decays with $\tau \sim 35$ ps have been measured for both $X_A$ and $X_B$ free excitons. For the thickest layer, the decay becomes biexponential with $\tau_1 \sim 80$ ps and $\tau_2 \sim 250$ ps. These values are preserved up to room temperature. By solving coupled rate equations in a four-level model, this evolution is interpreted in terms of the reduction of density of both shallow impurities and deep traps, versus layer thickness, roughly following a $L^{-1}$ law.

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**Study of High Quality AlN Layers Grown on Si(111) Substrates by Plasma-Assisted Molecular Beam Epitaxy**

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High quality AlN layers with full widths at half maximum values of 10 arcmin and average surface roughness (rms) of 48Å were grown by molecular beam epitaxy on Si(111) substrates. A systematic study and optimization of the growth conditions was performed in order to use these AlN layers as buffers in the growth of GaN films. Atomic force microscopy (AFM) and x-ray diffraction (XRD) techniques were employed to determine the surface and structural quality of the layers. Best AlN films were obtained at high substrate temperatures ($T_{subs} > 900$°C) and III/V ratios close to stoichiometry. Growth conditions with III/V ratios beyond stoichiometry (Al-rich) did not further improve the crystal quality. In these cases a higher substrate temperature is needed to prevent condensation of Al on the surface. GaN films with full width at half maximum of 10 arcmin and improved optical properties were grown on top of optimized AlN buffer layers.

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