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Effect of Magnesium and Silicon on the Lateral Overgrowth of GaN Patterned Substrates by Metal Organic Vapor Phase Epitaxy

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Metalorganic vapor phase epitaxy was used to achieve selective regrowth of undoped, Mg- and Si-doped GaN on a silicon nitride patterned mask, capping a GaN epitaxial layer deposited on (0001) sapphire substrate. Hexagonal openings in the mask defined into 10 μm diameter circles separated by 5 μm were used as a pattern for the present study. Uniform undoped and Mg-doped GaN hexagonal pyramids, delimited by C (0001) and R $\{1\bar{1}01\}$ facets, were achieved with a good selectivity. Si-doped GaN hexagonal pyramids delimited by vertical $\{1\bar{1}00\}$ facets and (0001) top facet were obtained for a high SiH_4 flow rate in the vapor phase. We found that the GaN growth rates V_R and V_C, measured in the R <1$\bar{1}$01> and C <0001> directions respectively, were drastically affected by the Mg and Si incorporation. By adjusting the Mg partial pressure in the growth chamber, the V_R/V_C ratio can be increased. Hence, the delimiting top C facet do not vanish as usually observed in undoped GaN selective regrowth but conversely expands. On the other hand, under proper growth conditions, 20-μm-high Si-doped GaN columns were obtained.

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Ultraviolet Photodetectors Based on $Al_xGa_{1-x}N$ Schottky Barriers

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Schottky barrier photovoltaic detectors based on Si-doped $Al_xGa_{1-x}N$ ($0 \leq x \leq 0.22$) have been fabricated and characterized. Samples were grown on basal plane sapphire by LP-MOVPE. Schottky contacts were made with Au. Responsivities are independent of the diode size and of the incident power in the range measured (10 mW/m$_2$ to 2 KW/m$_2$). The spectral response shows an abrupt cutoff that shifts linearly to higher energy with increasing Al content. A visible rejection of 3 to 4 orders of magnitude is observed in $Al_xGa_{1-x}N$ Schottky photodiodes. Device time response is RC-limited, and a minimum decay time as short as 15 ns have been estimated in unbiased $Al_{0.22}Ga_{0.28}N$ diodes. This time response can be further reduced by reverse biasing.

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Direct SIMS Determination of the $In_xGa_{1-x}N$ Mole Fraction

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We demonstrate that our secondary mass ion spectroscopy (SIMS) method for the determination of the mole fraction in solid $In_xGa_{1-x}N$ solutions is accurate and reproduceable without need of reference samples. The method is based on measuring relative current values of CsM^+ (M = Ga, In) secondary ions. The claim of reliable SIMS determination without reference samples was confirmed by four independent analytical methods on the same samples with a relative error in the InN mole fraction determination below 15%.

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The Polarity of GaN: A Critical Review

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GaN, AlN and InGaN have a polar wurtzite structure and epitaxial films of these materials typically grow along the polar axis. Although the polarity of these nitrides has been studied by quite a number of techniques, many results in the literature are in conflict. In this paper an attempt is made to lay out a set of polarity assignments to provide a context for discussion of these results. A "standard framework" is proposed to correlate the disparate results, and the framework is used to draw general conclusions about the polarity of bulk crystals, VPE and MBE epitaxial films, and devices.

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Surface Reconstruction During Molecular Beam Epitaxial Growth of GaN (0001)

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Surface reconstructions during homoepitaxial growth of GaN (0001) are studied using reflection high-energy electron diffraction and scanning tunneling microscopy. In agreement with previous workers, a distinct transi-

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tion from rough to smooth morphology is seen as a function of Ga to N ratio during growth. However, in contrast to some prior reports, no evidence for a 2 × 2 reconstruction *during* GaN growth is observed. Observations have been made using four different nitrogen plasma sources, with similar results in each case. A 2 × 2 structure of the surface can be obtained, but only during nitridation of the surface in the absence of a Ga flux.

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Selective Area Growth of GaN Directly on (0001) Sapphire by the HVPE Technique

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In this paper, we report on the selective area growth (SAG) of GaN directly on patterned *c*-plane sapphire substrates by hydride vapor phase epitaxy (HVPE). A number of researchers have reported that the HVPE growth technique, unlike the MBE and MOCVD methods, is capable of producing device quality GaN films without the need for any low temperature nucleation/buffer layers. The density of edge dislocations in these HVPE films decreases dramatically as the film thickness is increased, and the dislocation density values for thick films (> 10 μm) are comparable to those reported for the best GaN films grown by other methods on *c*-sapphire. These advantages of the HVPE growth technique makes it possible to achieve high quality selective area growth of GaN directly on *c*-sapphire substrates.

C-plane sapphire substrates were coated with PECVD SiO_2 and photolithographically patterned with different size and shape openings. Subsequently, these patterned substrates were introduced in a horizontal, hot-wall quartz reactor for the GaN growth. It was observed that single crystal GaN growth was preferentially initiated in the openings in the oxide layer. This selective area growth was followed by epitaxial lateral overgrowth (ELO), leading to the formation of hexagonal GaN prisms terminated in smooth, vertical $(1\bar{1}00)$ facets. We have been successful in shearing these pyramid structures from the sapphire substrates as individual devices, which do not require any post-growth etching for feature definition. This procedure allows for the dramatic reduction of the process complexity and the duration and expense for GaN growth for device applications. Stimulated emission results on these self-formed optical cavities are also presented.

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Surface Morphology of MBE-Grown GaN on GaAs(001) as Function of the N/Ga-Ratio

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Molecular beam epitaxy growth utilising an RF-plasma nitrogen source was used to study surface and surface morphology of GaN on GaAs (001) at 580°C. While both the nitrogen flow and plasma excitation power were constant, the grown layers were characterised as a function of Ga-flux. In the initial growth stage a (3 × 3) surface reconstruction was observed. This surface periodicity only lasted up to a maximum thickness of 2.5 ML, followed by a transition to the unreconstructed surface. Samples grown under N-rich, Ga-rich and stoichiometric conditions were characterised by high-resolution scanning electron microscopy and atomic force microscopy. We found that the smoothest surfaces were provided by the N/Ga-ratio giving the thickest layer at the (3 × 3)=>(1 × 1) transition. The defect formation at the GaN/GaAs interface also depended on the N/Ga-flux ratio.

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The Role of Piezoelectric Fields in GaN-Based Quantum Wells

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In this contribution, we focus on the consequences of the piezoelectric field, which is an inherent consequence of the commonly used wurtzite phase of GaN, on the optical properties of strained GaN-based quantum well structures. We demonstrate that both in GaN/AlGaN and in GaInN/GaN single quantum well structures, the piezoelectric field leads to a Stark-shift of the fundamental optical transitions, which can lead to luminescence emission far below the bulk bandgap. Due to the spatial separation of the electron and hole wavefunctions in such structures, the oscillator strength of these transitions may become extremely small, many orders of magnitude lower than in the field-free case. From specially designed structures, we can even determine the sign of the piezoelectric field and relate it to the polarity of the layers. Under high-excitation conditions, as found in a laser diode, the piezoelectric field is almost completely screened by the injected carriers. As a consequence, the stimulated emission is significantly blue-shifted compared to the photoluminescence, which has sometimes been confused with localization effects.

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Suppression of Phase Separation in InGaN Due to Elastic Strain

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The effect of elastic strain in epitaxial InGaN layers coherently grown on GaN wafers on spinodal decomposition of the ternary compound is examined. The effect results in considerable suppression of phase separation in the strained InGaN layers. To predict correctly the position of the miscibility gap in the T-*x* diagram it is important to take into account the compositional dependence of the elastic constants of the ternary compound. The contribution of the elastic strain to the Gibbs free energy of InGaN is calculated assuming uniform compression of the epitaxial layer with respect to the underlying GaN wafer. The interaction of binary constituents in the solid phase is accounted for on the base of regular solution model. The enthalpy of mixing is estimated using the Valence Force Field approximation. The strain effect becomes stronger with increasing In content in the InGaN. As a result the miscibility gap shifts remarkably into the area of higher InN concentration and becomes of asymmetrical shape. Various growth surface orientations and the type of crystalline structure (wurtzite or sphalerite) provide different effects of the elastic strain on phase separation in ternary compounds.

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Spectroscopic Ellipsometry on GaN: Comparison Between Hetero-Epitaxial Layers and Bulk Crystals

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In the present study spectroscopic ellipsometry was used for charactersing GaN bulk crystals obtained at high pressure and thin films grown on sapphire. The undoped GaN films grown by MOCVD show interference fringes below the fundamental gap. The ellipsometric data (Δ and Ψ), measured in the wavelength range between 500 nm and 680 nm, were analyzed using a multilayer description in the transfer matrix formalism. For the

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thin films grown on sapphire the model includes a buffer layer, a GaN epilayer, and a hypothetical overlayer. Furthermore, both, the real and imaginary part of the complex refractive index were taken into account. The real part of the refractive index n_1 was found to follow a Cauchy-type of dispersion $n_1 = 2.290 + 0.06\,[(280)/(\lambda\text{-}280)]^2$. For bulk crystals n_1 was found to be 2.337 (0.010 at the wavelength of 632.8 nm. This value compares well with MOCVD grown GaN where $n_1(\lambda = 632.8\text{ nm}) = 2.328 \pm 0.003$.

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Optical Properties of Electron-Irradiated GaN

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The electronic structure of defects produced by 2.5-MeV electron irradiation and their effect on optical properties of GaN are investigated using photoluminescence (PL) and optically detected magnetic resonance (ODMR) techniques. The electron irradiation is shown to produce, in particular, a deep PL band with a no-phonon line at around 0.88 eV followed by a phonon-assisted sideband. We suggest that this emission is caused by an internal transition between excited and ground state of a deep defect. The excited state is a multiple-level state, as revealed from temperature dependent PL and level anti-crossing experiments. The electronic structure of the 0.88 eV defect is shown to be sensitive to the internal strain in the GaN epilayers. The ODMR studies reveal that the principal axis of the defect coincides with the *c*-axis of the host lattice and should therefore be either an on-site point defect or an axial complex defect along the c-axis.

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Luminescence of Be-Doped GaN Layers Grown by Molecular Beam Epitaxy on Si (111)

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Low temperature photoluminescence spectra of Be-doped layers grown on Si (111) by molecular beam epitaxy have been analyzed. Emissions at 3.466 eV and 3.384 eV, and a broad band centered at 2.4-2.5 eV are observed. Their evolution with temperature and excitation power, and time resolved PL measurements ascribe an excitonic character for the luminescence at 3.466 eV, whereas the emission at 3.384 eV is associated with a donor-acceptor pair transition. This recombination involves residual donors and Be-related acceptors, which are located around 90 meV above the valence band, confirming Be as the shallowest acceptor reported in GaN. The intensity of the band at 2.4-2.5 eV increases with the Be content. This emission involves a band of deep acceptors generated by Be complex defects, as suggested by the parameter $g = 2.008 \pm 0.003$ obtained by photoluminescence-detected electron paramagnetic resonance.

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Mg-Enhanced Lateral Overgrowth of GaN on Patterned GaN/Sapphire Substrate by Selective Metal Organic Vapor Phase Epitaxy

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Selective and lateral overgrowth by Metal Organics Vapour Phase Epitaxy (MOVPE) was carried out until coalescence to produce smooth and optically flat thick GaN layers. A GaN epitaxial layer is first grown using atmospheric pressure Metalorganic Vapour Phase Epitaxy on a {0001} Al_2O_3 substrate. Then a 30Å silicon nitride dielectric film is deposited in-situ by reaction of silane and ammonia to form a selective mask. Afterwards, the openings and the figures in the dielectric films are achieved using standard photolithographic technology. Stripes openings in the mask, revealing free GaN surface, are aligned in the $<10\bar{1}0>$ direction. Typical stripes spacing and width are 10 µm and 5 µm respectively. These patterned layers are further on used for epitaxial regrowth of GaN by MOVPE. The growth anisotropy and therefore the coalescence process is achieved by introducing $(MeCp)_2Mg$ in the vapour phase. A two-step process is reported which allows a dramatic reduction of threading dislocations density not only above the masked areas but also above the windows opened in the mask. With this process, very sharp bound exciton luminescence peaks are measured at low temperature in the overgrown GaN.

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Polarization and Band Offsets of Stacking Faults in AlN and GaN

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We have performed systematic first-principles pseudopotential local density functional calculations of stacking faults in GaN and AlN. Their band offsets and the charge accumulation at stacking fault interfaces has been investigated, taking fully into account the effects of lattice relaxation and electric polarization. We find the stacking fault junctions to be of type I in both materials. However, the intrinsic valence band offsets are close to zero, so that the conduction band offsets result mostly from the differences in the energy gaps between the cubic and wurtzite phases. The charge accumulated at the interface between the cubic and wurtzite phase is found to be 0.009 and 0.003 C/m^2 for the AlN and GaN stacking fault, respectively.

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Time of Flight Mass Spectroscopy of Recoiled Ions Studies of Gallium Nitride Thin Film Deposition by Various Molecular Beam Epitaxial Methods

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Gallium Nitride (GaN) thin films were successfully grown by electron cyclotron resonance molecular beam epitaxy (ECR-MBE), gas source MBE (GSMBE), and chemical beam epitaxy (CBE). Time of flight mass spectroscopy of recoiled ions (TOF-MSRI) and reflection high energy electron diffraction (RHEED) were used *in-situ* to determine the surface composition, crystalline structure, and growth mode of GaN thin films deposited by the three MBE methods. The substrate nitridation and the buffer layers were monitored and optimized by TOF-MSRI and RHEED. For GSMBE, the gallium to nitrogen ratio is found to correlate well with *ex-situ* optical properties. In the case of CBE, carbon incorporation determines the surface morphology, crystalline quality and optical activity of the epilayers.

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High Quality GaN Films–Growth and Properties

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Growth of GaN/Al_2O_3 layers by MOVPE has been investigated. Precise optimization of the growth parameters results in films with extremely high electron mobility: 900 cm^2/Vs at 300K and 4000 cm^2/Vs at 77 K. The influence of the growth parameters on film properties like morphology, crystallographic structure, and the concentration of electrically active defects is presented. The mechanism of dislocation density reduction is proposed to explain the obtained results.

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