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editors@nsr.mij.mrs.org journalmaster@nsr.mij.mrs.org

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Analysis of the Visible and UV Electroluminescence in Homojunction GaN LED's

F. Calle[1], E. Monroy[1], F. J. Sánchez[1], E. Muñoz[1], B. Beaumont[2], S. Haffouz[2], M. Leroux[2], and P. Gibart[2]
[1]CiudadUniversitaria
[2]CRHEA-CNRS

The electrical and electroluminescent properties of MOVPE GaN *p-n* homojunctions have been analyzed as a function of temperature and bias. Electroluminescence is observed for V>3 V under dc and ac conditions. The main emission at low *T* is a donor-acceptor transition involving shallow acceptors, though it disappears at higher *T* due to the ionization of the acceptors and compensation by ionized donors. Room temperature dc and ac electroluminescence spectra evolve under increasing bias from a blue-shifting visible band involving deep states at the *p*-type side of the *p-n* junction, to a band-to-band uv recombination at high bias. In agreement, the superlinear dependence of light-current characteristics at low current injection becomes linear when the defects are saturated. Time analysis of the spectra vs pulse duration and duty cycle allows the determination of the visible radiative recombination and relaxation times associated to the Mg-related deep states, which are found to behave as acceptors lying 0.55 eV above the valence band. A simple 3-level model is able to explain the visible emission, which involves the conduction band (or shallow donor) and those deep acceptors in the *p*-layer. Optimum UV/visible ratio emission requires intense and relatively long pulses, with a high duty cycle to impede visible recombination.

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AMMONO Method of BN, AlN and GaN Synthesis and Crystal Growth

R. Dwilinski[1], R. Doradzinski[1], J. Garczynski[2], L. Sierzputowski[2], M. Palczewska[3], A. Wysmolek[1], and M. Kaminska[1]
[1]Warsaw University
[2]Warsaw Institute of Technology
[3]Institute of Electronic Materials Technology

Microcrystals of BN, AlN and GaN were obtained by the AMMONO method, in which nitridization of metal occurs in supercritical ammonia, at relatively low temperature and pressure conditions (below 550°C and 5 kbar). The reaction rate was regulated by the amount of mineralizers, i.e. alkali metal amides.

All crystals obtained by AMMONO method revealed intense and homogenous luminescence. Significant improvement of the optical properties was observed for crystals grown in the presence of Rare Earth elements. For such GaN crystals, helium temperature photoluminescence spectra were dominated by near-band-gap recombination. Exciton lines were extremely narrow, with full-width half-maximum (FWHM) as low as 1 meV. The concentration of uncompensated shallow donors in AMMONO GaN determined by electron paramagnetic resonance measurements was below 5×10^{15} cm^{-3}.

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Surface Structures, Surfactants and Diffusion at Cubic and Wurtzite GaN

T. Zywietz[1], J. Neugebauer[1], M. Scheffler[1], J. Northrup[2], and C.G. Van de Walle[2]
[1]Fritz-Haber-Institut der MPG
[2]Xerox–Palo Alto

Clean and As covered zinc-blende and wurtzite GaN surfaces have been investigated employing density-functional theory calculations. For clean GaN surfaces our calculations indicate the stability of several novel surface structures that are very different from those found on traditional III-V semiconductors. Adding impurities commonly present in significant concentrations during growth strongly modifies surface reconstructions and energies. In particular, we find that arsenic has a low solubility and significantly stabilizes the cubic GaN (001) surface making it interesting as a potential surfactant. Finally, we have studied the diffusion of Ga and N adatoms on both the equilibrium and non-equilibrium surfaces. Our calculations reveal a very different diffusivity for Ga and N adatoms: While Ga adatoms are very mobile at typical growth temperatures, the diffusion of N adatoms is slower by several orders of magnitude. These results give insight into the fundamental growth mechanisms and allow conclusions concerning optimum growth conditions.

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Structural Properties of MOVPE GaN Layers Grown By a New Multi-Buffer Approach

J. Kozlowski, R. Paszkiewicz, R. Korbutowicz, M. Panek, B. Paszkiewicz, and M. Tlaczala
Wroclaw University of Technology

GaN undoped layers of good morphology, good crystallinity and elec-

trical properties were grown on *c*-plane sapphire substrates by the atmospheric pressure MOVPE technique using a new multi-buffer growth approach. A suitable buffer layer growth technique was worked out which enabled growth of GaN layers with properties superior to those grown in a conventional process scheme. Additional buffer layers, deposited with increasing temperature and increasing V/III molar ratio, were inserted between the low temperature buffer layer and the high temperature GaN layer grown on it. The *c* and *a* lattice constants of the high temperature GaN overgrown layer were evaluated from x-ray data. The layer mosaicity and *c*-lattice parameter variation were determined. The relationship between *c* and *a* lattice parameters and the second buffer layer growth scheme has been studied. The effect of second buffer layer growth conditions, buffer layer annealing time as well as the influence of V/III molar ratio during the high temperature GaN deposition on the crystalline and electrical properties of overgrown GaN epitaxial layers are presented. Characterization includes surface morphology examination by SEM and Nomarski optical microscope, x-ray diffraction and *C-V* measurements.

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Heterostructure For UV LEDs Based on Thick AlGaN Layers

A.V. Sakharov, W.V. Lundin, A. Usikov, U. I. Ushakov, Yu.A. Kudriavtsev, A.V. Lunev, Y.M. Shemiakov, and N.N. Ledentsov
Ioffe Physical-Technical Institute

Thick AlGaN layers and GaN/AlGaN heterostructures were grown by low pressure MOCVD on (0001) sapphire substrates utilizing a low temperature AlGaN buffer layer. The distribution of Al in the thick AlGaN layers was observed to be non-uniform as a function of depth. The Al content gradually increases from the substrate towards the epilayer surface. Moreover, fluctuations of Al content are also noticeable. The saturation of impurity-related emission with increasing current density was observed in EL spectra of LEDs consisting of AlGaN/GaN/AlGaN DH sandwiched by a 2 μm-thick bottom layer of GaN:Si and 0.5 μm-thick layer of GaN:Mg. The dominant near-band edge emission of the GaN active layer was found to be strongly absorbed in the thick bottom layer. Utilizing a 2 μm-thick AlGaN bottom layer instead of the GaN one allowed the absorption edge to be shifted towards higher energies. A single peak at 362 nm with FWHM of 14 nm was observed in this type of LED. Luminescence properties of various types of heterostructures are also discussed.

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Optical Properties of GaNAs Grown by MBE

G. Pozina[1], I. G. Ivanov[1], B. Monemar[1], J.V. Thordson[2,3], and T.G. Andersson[2,3]
[1]Linköping University
[2]Chalmers University of Technology
[3]University of Göteborg–Sweden

Optical properties of the GaN_xAs_{1-x} layers grown on (001) GaAs substrates by molecular beam epitaxy have been studied. The samples can be classified into three categories with respect to the concentration of N, as determined by x-ray diffraction and secondary-ion mass spectrometry: (i) with doping nitrogen concentration, (ii) with average content of N less than 30%, and (iii) with *x* close to 100%. From optical measurements of photoluminescence and Raman scattering, combined with analysis of x-ray diffraction spectra, different phases are observed in the GaN_xAs_{1-x} layers: GaAs, GaN and the solid ternary solution GaN_xAs_{1-x}. We have estimated the fundamental band-gap energy in the GaN_xAs_{1-x} alloy with low nitrogen concentration (up to $x = 0.04$) from absorption measurements, and in GaN_xAs_{1-x} with low arsenic concentration (up to $1-x = 0.04$) from photoluminescence spectra. An analysis of the dependence of the experimental values of the GaN_xAs_{1-x} band-gap energy on the nitrogen composition indicates a constant bowing parameter *b* as large as $b = -18$ eV.

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Thermodynamic Properties of Group-III Nitrides and Related Species

I.N. Przhevalskii[1], S.Yu. Karpov[2], and Yu.N. Makarov[3]
[1]Russian Research Center
[2]Soft-Impact Ltd–Russia
[3]University of Erlangen-Nümberg

A database for thermodynamic properties of group-III nitrides and relevant species involved into growth of these materials is developed in this paper. Standard formation enthalpies of materials coefficients of polynomial approximations of the reduced Gibbs free energies are collected in the tables. They allow one to determine the Gibbs free energy, enthalpy, entropy and specific heat of a species as a function of temperature. The database covers solid and gaseous group-III nitrides, elemental species, gaseous metal-organic compounds, chlorides and hydrides of group-III elements, nitrogen containing precursors and organic byproducts of various chemical reactions proceeding during growth processes. Thermodynamic properties of adducts which can be formed in the vapor phase while mixing ammonia and metal-organic compounds are presented in the database as well. Much of the data given in this paper is presented for the first time. All the data are checked for self-consistency and therefore can be used for thermodynamic calculations.

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On the Bandstructure in GaInN/GaN Heterostructures–Strain, Band Gap and Piezoelectric Effect

C. Wetzel, S. Nitta, T. Takeuchi, S.Yamaguchi, H. Amano, and I. Akasaki
Meijo University

A study of the optoelectronic properties of strained 40 nm $Ga_{1-x}In_xN$ layers on GaN films is presented. The fact of pseudomorphic strain leads to a new interpretation of the film composition when derived from x-ray scattering. In addition we directly confirm that strain induces huge piezoelectric fields in this uniaxial system by the observation of Franz-Keldysh oscillations in photoreflection. As a function of composition ($0 < x < 0.2$) and strain we derive the electronic band gap energy and the piezoelectric field strength. We interpret both in terms of effective bowing parameters and piezoelectric coefficients, respectively. From a spatially resolved micro photoluminescence at room temperature we find no evidence for spatial band gap or composition variations of more than 60 meV over the length scale from 1 to 50 μm ($x = 0.187$) in our material. At the same time, an observed discrepancy between photoluminescence peak energy and photoreflection band gap energy increases with x to some 160 meV. We attribute this redshift to photon assisted tunneling in the huge piezoelectric fields (Franz-Keldysh effect).

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