HL 29: III-V Semiconductors I (mainly Nitrides)

Time: Tuesday 9:30–12:30 Location: EW 201

HL 29.1 Tue 9:30 EW 201

Coupled LO-Phonon-Plasmon Modes in Si- and Ge-doped GaN — •Max Bügler[1], Stephanie Fritze[2], Armin Dadgar[2], Alois Krost[2], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Magdeburg, Germany

Results of Raman spectroscopy on highly silicon and germanium doped GaN epilayers showing longitudinal-optical phonon-plasmon coupled modes are presented. Micro-Raman spectroscopy allows for spatially resolved probing of carrier concentration without the need to process electrical contacts. While it is inherently challenging to achieve high carrier concentrations ($>5{\cdot}10^{19}$cm^{-3}) in GaN by doping with Si, doping with Ge allows for carrier concentrations up to at least $2{\cdot}10^{20}$cm^{-3} without deterioration of the layers surface and crystalline quality. Raman spectroscopy is utilized to determine spatial fluctuations in the incorporation of Si and to proof homogeneity of doping by Ge. Results on films with carrier concentrations ranging from $3{\cdot}10^{18}$cm^{-3} to $6{\cdot}10^{19}$cm^{-3} for Si-doping and up to $2{\cdot}10^{20}$cm^{-3} for Ge-doping are presented. The observed dependence of the LPP^{-}-mode position on the carrier concentration is discussed and compared to theoretical predictions. To support the interpretation of the Raman results photoluminescence and photoluminescence excitation spectroscopy experiments are presented and discussed.

HL 29.2 Tue 9:45 EW 201

Influence of electron beam annealing on the structural and optical properties of GaN:Mg — •Christian Nenstiel[1,3], Marc Hoffmann[2,3], Trevor Manning[3], Gordon Callsen[1], Ramon Collazo[2], James Twiedie[2], Zlatko Sitar[2], Matthew Phillips[3], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]North Carolina State University, Materials Science and Engineering, USA — [3]University of Technology Sydney, Department of Physics and Advanced Materials, Australia

The chemical and structural origin of the in Magnesium doped GaN observed donor acceptor pair transitions (DAP) is not yet fully understood. Furthermore, the dynamics of Hydrogen during the commonly applied thermal activation process of MOCVD grown GaN:Mg are still a matter of active debate. To investigate these questions we grew 700 nm thick GaN:Mg layers. The samples exhibit Magnesium concentrations from 5E17 to 2E19 cm-3 and thermal annealing was before between 450 and 650 °C. Under electron beam exposure in CL measurements at 10 K we observed an increase of the intensity of the DAP luminescence until saturation after a few seconds which is then followed by rather complex shifting and quenching dynamics of the DAP luminescence. Additionally, we observed the quenching of acceptor bound excitons over time. None of these effects can be observed by Photoluminescence measurements , not even in the high excitation regime which allows us to derive electron beam induced technologically relevant dynamics of Hydrongen in GaN:Mg.

HL 29.3 Tue 10:00 EW 201

Surface states and band alignment of polar and nonpolar InN films studied by in-situ photoelectron spectroscopy — •Marcel Himmerlich, Anja Eisenhardt, and Stefan Krischok — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

The chemical and electronic properties of (0001), $(000\bar{1})$, $(1\bar{1}00)$ and $(11\bar{2}0)$ InN surfaces are analysed for stoichiometric and metal-rich growth conditions. Thin InN films were grown by PAMBE on GaN/Al_2O_3(0001), GaN/6H-SiC$(000\bar{1})$ and m/a-plane bulk GaN substrates, respectively, and characterised in-situ using XPS and UPS. The energy distance between surface valence band maximum and Fermi level (VBM-E_F) as well as the work function are dependent on crystal orientation. In general, In-rich growth leads to the formation of In adlayers which reduce VBM-E_F and result in the existence of a broad band of electron states inside the band gap. For stoichiometric $(000\bar{1})$, $(1\bar{1}00)$ and $(11\bar{2}0)$ InN surfaces, the band bending is strongly reduced compared to the (0001) configuration, pointing to nearly flat band conditions. The InN(0001) surface exhibits an In-induced (2×2) reconstruction and a surface state at the Fermi edge is detected, while for the growth on the other crystallographic orientations, no superstructure was formed and the occupied surface states are located at the valence band edge. The trends of variation of the surface band alignment as well as the observed occupied states agree with results of DFT calculations by D. Segev and C. G. Van de Walle (Europhys. Lett. 76, 305 (2006) & J. Appl. Phys. 101, 081704 (2007)).

HL 29.4 Tue 10:15 EW 201

Non-linear piezoelectric polarization in III-V semiconductors — •Pierre-Yves Prodhomme, Annie Beya-Wakata, and Gabriel Bester — Max-Planck Institut, Stuttgart, Deutschland

Piezoelectricity can be important for the electronic and optical properties of quantum well and quantum dots based devices such as lasers, light emitting diodes, infrared photodetectors. In particular it has been shown to be important in III-V and nitride semiconductors. The piezoelectric effect in quantum Well or in Quantum Dots is usually taken into account by neglecting the non linear term in the piezoelectric tensor. We have calculated the second order piezoelectric tensor for all the III-V (including the nitrides) semiconductors in the Wurtzite and Zincblende structure. And we have derived a relation between the proper and the improper second order piezoelectric coefficients. This relation is used to calculate the proper coefficients which are the experimentally measurable ones. We have calculated the piezoelectric field in several Quantum wells and compare our values to experiment. We show that the second order can be so large for Zinc-Blende materials that it cancels the first order term, we demonstrate also that for Nitrides this effect is much lower. However we show that for severely strained structure such as quantum dots or thin films, the second order piezoelectric effect can even exceed the spontaneous polarization in the nitrides.

HL 29.5 Tue 10:30 EW 201

Understanding and controlling In incorporation on InGaN surfaces: An ab initio approach — •Andrew Duff, Liverios Lymperakis, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Stra*β*e 1, 40237 Düsseldorf, Germany.

A first step in achieving full control on the growth and properties of $\{000\bar{1}\}$ (N-polar) InGaN surfaces is to gather a fundamental understanding of the relevant atomistic surface processes as well as to identify and investigate the differences in the growth of the N-polar face compared to the {0001} (Ga-polar) face. In this work, the incorporation of In into N- and Ga-polar surfaces is investigated using density functional theory (DFT) calculations. Total energies for an extensive range of reconstructions on the technologically relevant Ga-polar and N-polar surfaces are calculated and surface phase diagrams are constructed showing the most stable structures as a function of growth conditions. A substantially stronger binding for In adlayer/s and In adlayer/s with sub-surface In is found for N-polar compared to Ga-polar. Kinetic DFT calculations are also performed to address the competing effect of In segregation, with the surface segregation effect found to be weakest for the N-polar surface. Based on these results, the mechanisms of In incorporation, In segregation and also the self surfactant effect will be discussed in detail.

HL 29.6 Tue 10:45 EW 201

Excitonic effects and optical properties of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: A first-principle study — •Luiz Claudio de Carvalho, Jürgen Furthmüller, and Friedhelm Bechstedt — Institüt für Festkörpertheorie und -optiK, Max Wien Platz 1, 07743 Jena, Germany

Optical properties of group-III nitrides and of their alloys are of increasing interest. This holds especially for the emission properties in the so called green gap. A much deeper understanding of the interplay of clustering and composition fluctuations on the optical properties is needed. Random alloy and many-body theory can give an important contribution. In the present work, the optical properties and excitonic effects of wurtzite $In_xX_{1-x}N$ (X = Ga, Al) alloys and those of the end components are studied using a combination of methods. The alloys are described within the cluster expansion approximation. The optical spectra and the underlying excitonic effects are studied using a state-of-the-art treatment of the quasiparticle electronic structure and the solution of the Bethe-Salpeter equation (BSE). Explicitly we

use the Vienna Ab-initio Simulation Package (VASP) in order to compute the electronic structure for each local cation fraction. Based on the electronic structures, the BSE is solved and the optical absorption spectra, exciton binding energies, and electron-energy-loss spectra are computed and compared with available experimental data. At least, two different cluster statistics are investigated.

Coffee Break (15 min)

HL 29.7 Tue 11:15 EW 201

MOVPE growth of semi-polar GaN LED structures on planar Si(112) and Si(113) substrates — •Roghaiyeh Ravash, Armin Dadgar, Anja Dempewolf, Peter Veit, Thomas Hempel, Jürgen Bläsing, Jürgen Christen, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Fakultät für Naturwissenschaften,Universitätsplatz 2, 39106 Magdeburg, Germany

We present semi-polar GaN LED structures grown on non-patterned Si(112) and Si(113) substrates by MOVPE to improve light emitter efficiency. The samples were investigated by X-ray diffraction measurements, photoluminescence (PL), cathodoluminescence (CL) as well as field emission scanning electron microscopy (FE-SEM). In samples, which were simultaneously grown on Si(112) and Si(113), we observed that structures on Si(112) consist of a relatively smooth surface but those on Si(113) have a V-pit dominated surface with a three dimensional growth mode of the GaN layers resulting in a rough GaN surface. The low temperature CL spectra of the sample grown on Si(112) exhibit a dominant InGaN/GaN MQWs emission. But CL spectra of the MQWs grown on Si(113) show two peaks related to the rough surface resulting in inhomogeneous indium incorporation and / or thickness fluctuations in the MQWs. For an optimized sample grown on Si(113), the surface undulation of a first GaN layer is strongly reduced obtaining a LT-AlN interlayer nearly parallel to the substrate surface. There, CL measurements show only one dominant MQWs emission.

HL 29.8 Tue 11:30 EW 201

Surface atomic arrangements of polar (000-1) and semipolar (11-22) InN layers. — •Daria Skuridina, Sabine Alamé, Duc Dinh, Michael Kneissl, and Patrick Vogt — TU Berlin, Institute of Solid State Physics, Hardenbergstr. 36, EW6-1, 10623 Berlin, Germany

InN surface studies and their related electronic properties still lack a fundamental understanding, despite their great technological relevance. We performed surface studies on N-polar (000-1) InN layers grown directly on (0001) sapphire and semipolar (11-22) InN layers grown on (11-22) GaN templates by MOVPE. Morphology, atomic structure and surface symmetry of InN samples were measured by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED), respectively. Moreover, Auger electron spectroscopy was used for chemical composition analysis of the layers. The oxidized surfaces were annealed at 450°C under UHV conditions resulting in a significant reduction of the surface carbon and oxygen contaminations. Single atomic steps were observed on the clean (000-1) InN surface. Surface reconstruction (1x1) was observed by LEED and confirmed by the atom-resolved STM image. Scanning tunneling spectroscopy showed a metallic behavior on the N-polar InN that is in good agreement with predicted metal adlayer on the surface. The atomic arrangement of (11-22) InN layers showed no evidence of dimers or adatoms on the surface but the presence of In monolayer in agreement with the calculations by Yamashita et al. [1].

[1] Yamashita et al., Jpn. J. Appl. Phys. 48, 120201, (2009)

HL 29.9 Tue 11:45 EW 201

Growth of (20$\bar{2}$1) AlGaN, GaN and InGaN by metal organic vapor phase epitaxy — •S. Ploch[1], T. Wernicke[1], J. Rass[1], M. Pristovsek[1], M. Weyers[2], and M. Kneissl[1,2] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — [2]Ferdinand-Braun-Institut Leibniz Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

Green InGaN-based laser diodes on (20$\bar{2}$1) GaN substrates have recently demonstrated performances exceeding those of conventional (0001) oriented devices. However little is known regarding the growth parameters. We have investigated growth of AlGaN, GaN and InGaN on (20$\bar{2}$1) GaN substrates by MOVPE. Smooth GaN layers with a rms roughness <0.5 nm were obtained by low growth temperatures and reactor pressures. The layers exhibit undulations along [10$\bar{1}$4] similar to the GaN substrate. AlGaN and InGaN layers exhibit an increased surface roughness. Undulation bunching was observed and attributed to reduced adatom surface mobility due to the binding energy of Al and the low growth temperature for InGaN respectively or strain relaxation. AlGaN and InGaN heterostructures on (20$\bar{2}$1) GaN relax by layer tilt accompanied by formation of misfit dislocations, due to shear strain of the unit cell. This relaxation mechanism leads to a reduced critical layer thickness of (20$\bar{2}$1) AlGaN layers and InGaN multi quantum wells (MQW) in comparison to (0001). PL spectral broadening of 230 meV of (20$\bar{2}$1) InGaN single QWs emitting at 415 nm can be reduced by increased growth temperature or increased number of QWs with reduced thickness.

HL 29.10 Tue 12:00 EW 201

Active region design and MOVPE growth of UV–B light emitting diodes — •F. Mehnke, J. Stellmach, T. Kolbe, M.-A. Rothe, C. Reich, T. Wernicke, M. Pristovsek, and M. Kneissl — Institute of Solid State Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The external quantum efficiency of AlGaN–based ultraviolet (UV) light emitting diodes (LED) decreases with shorter emission wavelength. This is attributed to a higher defect density, carrier localization, increased magnesium acceptor ionization energy and an enhanced incorporation of impurities.

We studied the influence of active region and electron blocking layer (EBL) design on the injection efficiency. UV LEDs were grown by metalorganic vapour phase epitaxy (MOVPE) in a spectral range between 320 nm and 290 nm. The devices were characterized by electro– and photoluminescence spectroscopy and XRD. With increasing aluminium content in the active region i.e. decreasing emission wavelength we observe for an $Al_{0.6}Ga_{0.4}N$ EBL a decrease of output power and increase of p–side luminescence. This indicates decreasing injection–efficiency due to a lower effective barrier height of the EBL. We will discuss the effect of the barrier height and magnesium doping on the injection efficiency and compare the results with 1D–drift–diffusion simulation.

HL 29.11 Tue 12:15 EW 201

Crystal field investigations of rare earth doped aluminum nitride — •Ulrich Vetter[1], Tristan Koppe[1], Takashi Taniguchi[2], John B. Gruber[3], Gary W. Burdick[4], and Hans Hofsäss[1] — [1]2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]National Institute for Materials Science, Namiki 1 - 1, Tsukuba, Ibaraki 305-0044, Japan — [3]Department of Physics and Astronomy, The University of Texas at San Antonio, San Antonio, 4 Texas 78249-0697, USA — [4]Department of Physics, Andrews University, Berrien Springs, Michigan 49104-0380, USA

Aluminum nitride belongs to the most promising semiconducting rare earth hosts due to its large band gap of around 6.2 eV and its high thermal conductivity, thus showing properties which make it useful for high power light emitting devices. In this work we are comparing the optical properties of aluminum nitride doped with rare earths during high-temperature, high-pressure synthesis to aluminum nitride doped by ion implantation, in detail considering the crystal field analyses for selected rare earth ions. Additionally the influence of co-doping with e.g. oxygen and fluorine on the optical properties of the host matrix and the rare earth intra-4f electron transitions is discussed, together with issues regarding electrical contacts.