HL 1: Nitrides: Preparation and characterization I

Time: Monday 9:30–13:00 Location: EW 015

HL 1.1 Mon 9:30 EW 015

Time-resolved ellipsometry on degenerately doped cubic GaN — •Elias Baron[1], Rüdiger Goldhahn[1], Michael Deppe[2], Donat J. As[2], Shirly Espinoza[3], Martin Zahradník[3], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany — [3]ELI Beamlines, ELI ERIC, Dolní Břežany, Czech Republic

The interest in ultra-fast processes in semiconductors has steadily increased in recent years, as modern technologies require faster and faster electronics and optics. Highly sensitive measurement techniques are essential for researching these phenomenons. In this context, time-resolved spectroscopic ellipsometry (TRSE) proved to be an excellent technique for determining the transient optical properties. Additionally, the metastable cubic phase of the well-known GaN offers advantageous properties for investigating fundamental processes in excited semiconductors. We present our analysis of thin film cubic GaN, deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation and doped by either Ge or Si up to $9\times10^{19}\,\mathrm{cm}^{-3}$. TRSE measurements, based on a pump-probe approach in the UV spectral range are performed using a 266 nm pump-beam. The electron-hole pairs generated by this pump-beam influence the optical properties due to many-body effects like band gap renormalization and Burstein-Moss shift. The impact of these effects vary depending on the doping concentration. Furthermore, a free-carrier profile from top to bottom has to be considered for an accurate description.

HL 1.2 Mon 9:45 EW 015

Optical properties of cubic $In_xGa_{1-x}N$ thin films — •Jonas Rose[1], Elias Baron[1], Rüdiger Goldhahn[1], Mario Zscherp[2], Silas A. Jentsch[2], Sangam Chatterjee[2], Jörg Schörmann[2], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

Cubic InGaN (c-InGaN) is a promising material for fabricating highly efficient optoelectronical devices and can potentially replace its hexagonal counterpart for certain applications. Due to the lack of internal polarization fields and lower band gap energies c-InGaN is a suitable candidate for applications in the visible spectrum. Especially InGaN/GaN quantum wells can be used for green light-emitting devices. Therefore, the knowledge of its optical properties is of special interest. In this context, spectroscopic ellipsometry is a sophisticated experimental technique due to its high sensitivity as well as contact- and destruction-free operation. Recently, several breakthroughs in crystal growth regarding structural quality and range of In-content have been achieved.

We present our investigation of c-InGaN thin films deposited by plasma-assisted molecular beam epitaxy (MBE) on 3C-SiC/Si substrates in (001) orientation. Spectroscopic ellipsometry measurements in the IR and VIS-UV spectral range yield the dielectric function containing phonon and plasmon contributions as well as interband transitions. Additionally, many-body effects affecting the absorption edge are taken into account.

HL 1.3 Mon 10:00 EW 015

Time-resolved cathodoluminescence spectroscopy of oxygen related defects in AlN layers — •Barbara Szafranski, Lukas Peters, Andreas Waag, and Tobias Voss — Institute of Semiconductor Technology, Braunschweig University of Technology, Germany

High temperature annealing (HTA) of sputtered AlN leads to a substantial improvement of the crystal quality. However, during the annealing process, a large number of point defects like oxygen is introduced. Oxygen has a double-edged role during HTA.

We therefore analyzed oxygen defects in AlN layers with cathodoluminescence (CL) spectroscopy. The 350 nm thick AlN layers were treated with HTA at different temperatures. The process has been optimised to lead to very high crystal quality.

At room temperature, CL spectroscopy shows a broad (FWHM 650 meV) luminescence band centered at about 3.66 eV (340 nm), which we correlate with oxygen point defects. To study the charge carrier dynamics of these defects in AlN, time-resolved CL measurements have been performed. The defect related emission is characterized by a complex multiexponential decay with a fast component of about 1 ns and a slow component of tens to hundreds of nanoseconds. In agreement with Genji et al., we attribute the short decay time to the radiative transition from the conduction band-edge states to $(V_{Al}-2O_N)^{1-}$ and $(V_{Al}-O_N)^{2-}$ and the long decay times to trapping and detrapping processes of the charge carriers via shallow traps [1].

[1] Kumihiro Genji and Takashi Uchino, Appl. Phys. Lett. 109, 021113 (2016).

HL 1.4 Mon 10:15 EW 015

n-type doping of GaN via pulsed sputter epitaxy — •Florian Hörich, Jürgen Bläsing, Jona Grümbel, Martin Feneberg, Rüdiger Goldhahn, Armin Dadgar, and André Strittmatter — Otto-von-Guericke University

Semiconductor devices like HEMTs typically employ a highly insulating buffer and a current transport layer. Recent developments in reactive sputter epitaxy have led to high resistances and breakdown field strenghs for GaN /1/. This talk focusses on n-type doping of GaN via co-sputtering with Si and Ge. For both dopants carrier concentrations ranging from 10^{17} up to 10^{20} cm^{-3} are feasible. The carrier density evaluated by Hall-effect and by PL measurements, evaluated for the free-carrier concentration by the bandgap shift (Burstein-Moss effect) /2/, are in good agreement. Just like MOVPE grown layers, highly Si doped layers tend to surface roughening due to SiN formation. This effect is even more pronounced for Ge doped layers. The relatively low growth temperature of 750 °C likely promotes Ge_xN_y formation. Contrary to MOVPE results, XRD measurements show an additional peak in the $\theta/2\theta$-Scan for Ge doped layers, indicating a distortion of the lattice.

/1/ A. Dadgar et al, Phys. Stat. Sol. a 220, 2200609 (2022) /2/ M. Feneberg et al. Physical Review B 90, 075203397 (2014)

HL 1.5 Mon 10:30 EW 015

Bandgap Engineering in Cubic Nitrides: a Theoretical Study — •Jan M. Waack[1,2], Markus Kremer[1,2], Nils Andre Schäfer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

For new applications like integrated RGB LEDs, a precise bandgap engineering over the full visible spectrum is desired. This can be achieved by alloying a narrow bandgap material such as indium nitride (InN) or scandium nitride (ScN) with a wide bandgap semiconductor such as gallium nitride (GaN) or aluminum nitride (AlN).

These material systems like (Al,Sc)N or (In,Ga)N are random alloys that require specific techniques such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2] to ensure accurate calculations. To properly predict the fundamental electronic band gap, we use the low computational cost LDA-1/2 method [3]. In this study, we present our results on structural and electronic properties such as stability, lattice parameter, band gap and phonon modes.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). https://doi.org/10.1103/PhysRevB.88.094421

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. 65, 353 (1990). https://doi.org/10.1103/PhysRevLett.65.353

[3] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). https://doi.org/10.1103/PhysRevB.78.125116

HL 1.6 Mon 10:45 EW 015

deciphering the origin of small pits in GaInN/GaN quantum wells structures: correlation of defect formation and growth conditions — •Mahdi Khalili Heyarjaribi[1,2], Rodrigo de Vasconcellos Lourenço[1,2], Uwe Rossow[1,2], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

Threading dislocations are non-radiative centers and can affect the luminescence efficiency of light emitters based on GaInN/GaN quantum wells (QWs).Specially for heteroepitaxial growth,i.e on sapphire substrate, the dislocation density is high, leading to a significantly reduced

luminescence efficiency. This issue can be addressed by intentionally creating V-pits, screening the threading dislocations cores. We have observed that sometimes additional pits are visible after the growth of the quantum well stack. Those pits are far smaller in size and usually appear as pairs, and may be associated to defects, e.g. stacking faults, which are formed during QW growth and may act as non-radiative centers. Employing scanning electron microscope (SEM) imagery, we investigate the V-pits. The analysis of thousands of images is a very time consuming and laborious procedure. We developed a model, using YOLO machine learning algorithm, which can objectively characterize the pits,their size distribution, density, and can selectively focus on the small pits.The trained model is more efficient and faster than conventional methods.Using the results and systematic variations of structural parameters, we elucidate the origin of the small pits.

15 min. break

Invited Talk HL 1.7 Mon 11:15 EW 015

Strong light-matter interaction probed by cathodoluminescence spectroscopy — •Fatemeh Chahshouri[1] and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel, Nano, Surface, and Interface Science -KiNSIS, Kiel University, 24098 Kiel, Germany

Electron microscopy is a powerful tool that offers detailed views of a composition of biological, chemical, and semiconductor structures with atomic-scale resolution. Additionally, it enables us to study quantum phenomena at the nanoscale and explore exciting phenomena, such as probing (quantum-)optical excitation and tailoring the shape of electron beams, where the latter further allows for more advanced characterization techniques. In this talk, we will discuss the functionality of cathodoluminescence spectroscopy in investigating the formation and propagation of exciton-polaritons in van der Waals materials. We will further discuss how generated secondary electron carriers in the heterostructure of group III nitride materials can interact with defects and Schottky barriers and generated two-dimensional electron gas inside the heterojunction. Furthermore, we will describe our numerical investigations on modulating and shaping the electron wavepacket after interacting with laser-induced optical near-fields in the vicinity of the material. Our work introduces new possibilities, allowing electrons to be utilized as a nanoscale source for probing matter and opens up avenues for improving state-of-the-art electron microscopy through the use of tunable electron beams in enhancing the electron beam interaction with light and matter.

HL 1.8 Mon 11:45 EW 015

HAXPES Study of $Al_{1-x}Sc_xN$-based Ferroelectric Capacitors — •Oliver Rehm[1], Lutz Baumgarten[2], Roberto Guido[3], Pia Düring[1], Andrei Gloskovskii[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[1] — [1]Uni Konstanz, Konstanz, Germany — [2]FZJ, Jülich, Germany — [3]NaMLab, Dresden, Germany — [4]DESY, Hamburg, Germany — [5]TU Dresden, Dresden, Germany

The novel ferroelectric (FE) material $Al_{1-x}Sc_xN$ exhibits a large remanent polarization and coercive field, with huge potential for the next generation of nonvolatile memory devices. However, the application of AlScN-based thin films as active FE is currently hampered by cycling endurance and leakage issues, which are worse than that of HfO_2.

The present work focuses on exploring the chemical properties of $Al_{0.83}Sc_{0.17}N$ thin films (60 nm) using hard x-ray photoelectron spectroscopy (HAXPES). Studying both W-capped and uncapped samples, we show that AlScN is not stable in air due to surface-enhanced oxidation over long periods (weeks to months). By comparing the contribution of Sc and Al relative to the overall oxidation of $Al_{1-x}Sc_xN$, we assume that oxygen tends to occupy a neighbour lattice site of Sc, resulting in an enhanced oxidation of Sc compared to Al. Moreover, the oxidation process causes N atoms to be removed from their lattice sites, likely leading to an incorporation of interstitial N, which is deduced from the observation of a surface-enhanced spectral feature of the N 1s core-level.

O. Rehm, L. Baumgarten, M. Müller et al., in preparation

HL 1.9 Mon 12:00 EW 015

Multiphonon Raman scattering in rocksalt ScN — •Stefan Wolf[1], Jona Grümbel[1], Yuichi Oshima[2], Christopher Lüttich[1], Florian Hörich[1], Armin Dadgar[1], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität, Universitätsplatz 2, 39106, Magdeburg — [2]Research Center for Electronic and Optical Materials, National Institute for Materials Science , 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

We investigate rocksalt ScN films with different free carrier concentration using Raman spectroscopy. Two different sets of samples were used for our measurements: (I) ca. 300nm thick ScN grown by sputter epitaxy and (II) 0.4 μm up to 40 μm thick ScN grown by HVPE. The HVPE grown ScN exhibits a very good crystalline structure, with carrier concentration varying between $10^{18}cm^{-3}$ and $10^{20}cm^{-3}$, while for ScN grown by sputter epitaxy, the carrier concentrations even reach $10^{21}cm^{-3}$ or more. We obtain detailed information about the impact of free carriers on coupled optical phonon-plasmon (LPP) modes up to a scattering order of $n_{LPP} = 3$.

The observed frequency shift of the first and second order LPP modes with respect to the carrier concentration shows an overdamped behaviour, indicating strong electron-electron interaction. As expected, transverse optical phonon modes show no significant frequency shift over the whole carrier concentration range. Correct assignment of multiphonon lines and possible future steps in understanding their behaviour will be discussed.

HL 1.10 Mon 12:15 EW 015

Point defect diffusion in GaInN/GaN quantum well structures — •Rodrigo De Vasconcellos Lourenco, Philipp Henning, Philipp Horenburg, Uwe Rossow, Heiko Bremers, and Andreas Hangleiter — Institute of Applied Physics, Technische Universität Braunschweig, Germany

A reduction of the point defect density in light-emitters based on GaInN/GaN quantum wells (QW) is desired for maximising the internal quantum efficiency. We investigate the non-radiative lifetime of GaInN/GaN single QWs grown on In-free and In-containing underlayers (UL). The non-radiative lifetime of SQWs increases with UL thickness in both cases. Since the non-radiative lifetime is inversely proportional to the defect density and as V-pits efficiently suppress the recombination at threading dislocations, our result suggests a point defect density profile over distance between the high temperature GaN buffer layer and the QW. Hence, a simple solution to the diffusion equation allows to accurately fit our data and yields a defect diffusion coefficient. point defect diffusion is a thermally activated process, associated with a defect migration barrier, which is in the range expected for the nitrogen vacancy in n-type GaN. Surprisingly, an attempt to reproduce the results lead to non-radiative lifetimes about one order of magnitude lower than previously, but with the same activation energy. This means that diffusion is prevalent in the same way, but with a different boundary condition, i.e. a higher density of point defects in the underlying GaN buffer.

HL 1.11 Mon 12:30 EW 015

Phases of sputtered Hf_xN_y: XRD, Ellipsometry and Raman spectroscopy studies — •Jona Grümbel, Christopher Lüttich, Jürgen Bläsing, Armin Dadgar, Martin Feneberg, and Rüdiger Goldhahn — Otto-von-Guericke-Universität, Universitätsplatz 2, 39106, Magdeburg,

Several phases of the binary material system Hf_xN_y are predicted to be stable or metastable, where the thermodynamically preferred rocksalt ($Fm\bar{3}m$) structured HfN exhibits the lowest formation energy and a metallic character. The metastable modified zincblende like ($I4\bar{3}d$) structured Hf_3N_4 is predicted to be semiconducting. Aiming for metallic rs-HfN, various samples were prepared via DC magnetron sputtering under varying conditions, e.g. using N_2 or N_2+NH_3 as sputter gases. Surprisingly, samples with high ammonia flow (>10 sccm) lose their golden metallic color but exhibit typical thin film interference colors, indicating transparency in the visible spectral range. We apply UV ellipsometry and Raman spectroscopy measurements to proof, that Hf_xN_y grown with increasing ammonia flux becomes semiconducting with an absoprtion edge of ≈ 3 eV. Annealing metallic HfN samples under ammonia atmosphere yields the same semiconductiong Hf_xN_y phase with several narow Raman bands and an absorption edge of ≈ 3 eV as well. Surprisingly, XRD powder diffraction indicates a new phase only for the annealed sample. Detailed analysis of the optical characteristics will be presented as well as a comparison to various theroretical calculations of different Hf_xN_y phases.

HL 1.12 Mon 12:45 EW 015

Highly resolved cathodoluminescence spectra of N-polar homoepitaxial AlN — •Domenik Spallek[1], Gwénolé Jacopin[2], Len van Deurzen[3], Jashan Singhal[3], Jimy Encomendero[3], Oliver Brandt[1], Debdeep Jena[3], and Jonas Lähnemann[3] —

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As a semiconductor with an ultra-wide band gap, AlN is an interesting material for applications in optoelectronic devices such as UV-LEDs. Additionally, its high thermal conductivity and breakdown field are advantageous for applications in high power electronics. High quality AlN layers of either Al or N polarity can be grown homoepitaxially on commercial substrates by molecular beam epitaxy (MBE) [1]. Besides serving as potential basis for device structures, the low point defect and dislocation densities result in high luminous efficiencies, which makes such layers a suitable platform for comprehensive investigation of their fundamental excitonic emission.

We focus on an N-polar AlN layer and present near-band-edge cathodoluminescence spectra as a function of temperature, as well as for different measurement geometries. An improved spectral resolution uncovers additional emission lines compared with Ref. 1. The various emission lines can be assigned to free excitons with different symmetries and defect-bound states of different origin, as well as their phonon replicas. Thus, this study contributes to the resolution of controversies in the attribution of excitonic emission lines in AlN.

[1] van Deurzen *et al.*, APL Mater. **11**, 081109 (2023)