

HL 33: Poster Session III

Time: Wednesday 17:30–19:30

Location: Poster F

HL 33.1 Wed 17:30 Poster F

Investigation of the effects of Mg-doping on the structural and electrical properties of (In,Ga)N/GaN superlattices —

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Optimization of the p-type area is one of the challenges for the realization of more efficient light emitters based on group III-nitrides. A self-compensation mechanism limits the hole density in the Mg-doped (In, Ga)N layers usually constituting the p-type area. Instead of directly increasing the hole concentration on the topmost contact layer, the hole injection may be promoted by utilizing (In, Ga)N/GaN superlattices (SLs) neighboring the active region. To this aim, we investigate the influence of Mg on the structural and electrical properties of (In, Ga)N/GaN SLs and (In, Ga)N layers grown by PAMBE. SL samples with 10 periods of (In, Ga)N/GaN were fabricated at 610°C and doped with Mg at different steps of the period. In-situ monitoring of the In desorption by QMS indicated a decrease in In incorporation in the SLs with the amount of Mg supplied. XRD was employed to assess this effect, as well as the structural quality of the SLs. Significant improvement of the surface morphology was achieved by the SL formation compared to the random alloy. In addition, the electrical characterization confirmed the p-type nature of some of the SLs. Our results pave the way for improved hole injection efficiency in III-N emitters.

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HL 33.2 Wed 17:30 Poster F

Band offset at the Ga(N,As,P)/GaP Heterointerface —

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The realization of monolithically integrated on-chip laser sources for optical data transmission remains to be one of the major goals of optoelectronic integration. The quaternary III-V material system Ga(N,As,P) promises to fulfil this task. Composition variations through the control of nitrogen and phosphorous incorporation allow for both, bandgap engineering, potentially covering the near-infrared regime as well as the telecom wavelength and matching the lattice constant to Si. Here, we investigate a series of Ga(N,As,P) multiple quantum well samples. The well thickness is varied while the composition is kept quasi-constant. The samples are examined by photoluminescence excitation spectroscopy. Besides higher states, we find two clear peaks slightly above the band-gap energy, which we attribute to the heavy-hole and light-hole valence band to conduction band energy transitions of the samples. Consequently, we are able to model the band offset at the Ga(N,As,P)/GaP heterointerface with a band anti-crossing model and the model solid theory.

HL 33.3 Wed 17:30 Poster F

Characterization of electro-chemical treated GaN-Nanowires —

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Due to its large surface to volume ratio GaN nanowires show excellent properties for bio-sensing and water-splitting applications. Therefore, the optical, structural and electrochemical properties of photo-electrochemically treated and untreated GaN nanowires were investigated. The GaN nanowires ensembles were immersed in an aqueous phosphate buffered saline solution (PBS) and treated under various bias and illumination conditions. Photoluminescence measurements show that anodic biases induce a permanent decrease in the radiative recombination intensity. The structural properties of the treated samples changed from free standing nanowires to more tilted structures,

as can be seen in scanning microscopy images. We find that the effects are stronger for higher anodic biases and longer treatment times. Energy dispersive x-ray spectroscopy shows that the surface of the nitride nanowires is oxidized as a consequence of the treatments.

HL 33.4 Wed 17:30 Poster F

Raman spectroscopic characterization of GaN grown by high-temperature vapor phase epitaxy —

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High-temperature vapor phase epitaxy (HTVPE) [1] is considered as a cost-efficient technology for fabrication of GaN templates. In this work, recent results on structural and optical characterization of GaN layers grown by HTVPE at various growth conditions will be presented. Analysing reciprocal space maps recorded by HRXRD, the threading dislocation density of the investigated samples was assessed. In order to monitor residual stress within the GaN layers confocal Raman spectroscopic measurements at room temperature with high lateral and spatial resolution were performed. The spectral position of the non-polar E₂(high) Raman mode indicates compressive in-plane strain, which is reduced with increasing GaN layer thickness. This work is financially supported by the European Union (European Social Fund) and by the Saxonian Government (grant no. 100231954).

[1] G. Lukin et al. Phys. Stat. Solidi A **65** (2017) 1600753

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Cathodoluminescence characterization of stacking faults in GaN —

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Semipolar GaN samples, heteroepitaxially grown by metal organic vapor phase epitaxy on pre-structured sapphire substrates, are possible substrates for efficient optoelectronic devices. Due to the sophisticated growth mode on pre-structured sapphire substrates, defects in the epitaxial GaN layer are formed. These include basal plane stacking faults in various types, such as I₁, I₂ and terminating prismatic dislocations. Mostly, these defects are created at an early stage of growth, but also they form during coalescence.

In this study we present spatially and spectrally resolved low-temperature cathodoluminescence (SEM-CL) investigations from a semipolar coalesced (10 $\bar{1}$) GaN sample, grown on a pre-structured r-plane sapphire substrate. This sample shows complex luminescence signatures from several types of crystal defects.

HL 33.6 Wed 17:30 Poster F

Polarisation resolved PL-studies of thin AlBGaIn-layers —

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We try to incorporate small amounts of boron into AlGaIn to reduce the lattice mismatch to AlN. This enables strain management in the material system and should help to reduce the quantum confined Stark effect in quantum well structures, hence increasing the external quantum efficiencies of UV-LEDs. However, strain reduction can also have negative impact. By inverting the valence band order and thus switching the emission from TE to TM Mode. In the ternary compound AlGaIn, this polarisation switching occurs at a specific composition, which is strongly strain dependent. For high Al content, for which the TM-

polarisation is predominant, higher strain enhances TE polarisation. To study the influence of boron on strain and polarisation, mainly optical spectroscopy and X-Ray diffractometry were used, alongside with other characterisation methods. Even for reduced strain, enhanced TE polarisation was observed for boron containing samples.

HL 33.7 Wed 17:30 Poster F

Determination of polarization fields in group III-nitride heterostructures by capacitance-voltage measurements — ●MARCEL SCHILLING, NORMAN SUSILO, LUCA SULMONI, MARTIN GUTTMANN, TIM WERNICKE, and MICHAEL KNESSL — Technische Universität Berlin, Institute of Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany

Due to changes in the spontaneous and piezoelectric polarization, group III-nitride heterostructures exhibit strong polarization fields at heterointerfaces in the order of MV/cm. For quantum wells, the polarization fields lead to a strong band bending and a redshift of the emission wavelength, known as quantum-confined Stark effect. In order to study the influence of polarization fields in group III-nitride-based semiconductor devices, an accurate determination of the magnitude and direction of the polarization fields is of great importance.

We demonstrate a new method to precisely determine the polarization fields in group III-nitride heterostructures based on capacitance-voltage measurements. By evaluating the changes in the depletion region width of a pin diode or Schottky diode, we are able to determine the polarization fields with high accuracy. For this approach, it is necessary to compare the depletion region width of a reference sample without the heterostructure (i.e. homojunction) to a sample with a quantum well structure. Finally, we will discuss the accuracy and possible sources of errors for this method.

HL 33.8 Wed 17:30 Poster F

Optical properties of metamorphic semipolar group III-nitride quantum well structures — ●DANIEL SCHMID¹, PHILIPP HENNING¹, PHILIPP HORENBURG¹, FEDOR ALEXEJ KETZER¹, HEIKO BREMERS¹, UWE ROSSOW¹, FLORIAN TENDILLE², PHILIPPE DE MIERRY², PHILIPPE VENNÉGUÈS², JESÚS ZÚÑIGA-PÉREZ², and ANDREAS HANGLEITER¹ — ¹Institut für Angewandte Physik, Technische Universität Braunschweig — ²Centre de Recherche sur l'Hétéro-Epitaxie, Valbonne, France

In this contribution we discuss the carrier dynamics in semipolar (11 $\bar{2}$) quantum well structures. In particular we study the influence of reduced strain in metamorphic structures on recombination processes. For this purpose we control the strain of our samples with AlInN buffer layers to adjust our lattice parameters. Via temperature dependent time-resolved photoluminescence we took a deeper look into the relation between radiative and nonradiative recombination processes of thin (1.5 nm) metamorphic semipolar (11 $\bar{2}$) GaInN/GaN MQW structures. Our samples were grown with low pressure MOVPE on high quality pseudo bulk GaN substrates as well as on templates grown on patterned sapphire. We measured radiative lifetime of 0.32 ns at 5 K and 1.44 ns at RT. The non radiative lifetime of the sample grown on pseudo bulk GaN was higher compared to samples grown on patterned sapphire, which leads to the idea of fewer defects inside the QW and therefore less non radiative recombination centres. In addition we discuss the effect of the band structure as derived by $\mathbf{k} \cdot \mathbf{p}$ calculations.

HL 33.9 Wed 17:30 Poster F

Transport properties and structural characteristics of thin AlGaIn/(AlN)/GaIn heterostructures and their built-in 2D electron gases — ●DENNIS MAUCH, HEIKO BREMERS, UWE ROSSOW, and ANDREAS HANGLEITER — Institut für Angewandte Physik, TU Braunschweig, Germany

We present transport properties of ultrathin AlGaIn/AlN/GaN heterostructures, grown on c-oriented sapphire substrates in our commercial MOVPE system. These heterostructures form a two-dimensional electron gas (2DEG) with high mobilities, showing values exceeding 15000 cm²/Vs at 4K with observed sheet carrier densities ranging from 3 – 12 × 10¹² cm⁻². As a consequence of the noncentrosymmetry of the wurtzite structure in group-III nitrides, a large spontaneous polarization is oriented along the hexagonal c-axis. In addition, group-III nitrides are highly piezoelectric. Hence, in AlGaIn/GaN heterostructures, where the AlGaIn layer is grown pseudomorphically on top of GaN, strain leads to piezoelectric polarization in this AlGaIn epitaxial layer. The electric field, induced by the polarization discontinuity at the heterointerface, then gives rise to the formation of a 2DEG ("polarization doping"). We also investigated the influence of an additional

AlN interlayer at the AlGaIn/GaN interface in order to reduce alloy disorder scattering and thus to reach higher 2DEG mobilities. The transport properties were analysed via Hall effect measurements at room temperature and also by Shubnikov-de Haas measurements at 4K. The structural details were obtained from high-resolution X-ray diffraction and X-ray reflectivity.

HL 33.10 Wed 17:30 Poster F

Investigation of the optical polarization of AlGaIn multiple quantum wells using photoluminescence spectroscopy — ●BETTINA NEUSCHULZ¹, CHRISTOPH REICH¹, JOHANNES ENSLIN¹, BARAN AVINC¹, FRANK MEHNKE¹, NORMAN SUSILO¹, CHRISTIAN KUHN¹, TIM WERNICKE¹, and MICHAEL KNESSL^{1,2} — ¹Technische Universität Berlin, Institute of Solid State Physics — ²Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

The valence band order in AlGaIn quantum wells (QW) is strongly affected by the aluminum mole fractions in QW (x) and barrier (y) as well as the QW width. This can lead to a switching of the polarization $P = (TE - TM)/(TE + TM)$ of the emitted light from mainly transverse-electric (TE) to transverse-magnetic (TM). The symmetry and order of the respective valence bands can be probed by polarization resolved photoluminescence (PL) as the degree of optical polarization is directly linked to the valence band properties. Using PL spectroscopy, the optical polarization of the in-plane AlGaIn QW emission at room temperature has been investigated, and in a systematic study, the aluminum mole fractions of the QWs and barriers as well as the QW width have been varied. Measurements show that for 1.5 nm thin Al_xGaN/AlN QWs the degree of polarization is changing from 0.33 (TE) for $x = 0.6$ to -0.13 (TM) for $x = 0.81$. Using 2 nm wide QWs with $x = 0.6$ and $y = 0.81$ strongly TE polarized light $P = 0.7$ can be obtained. The transition from TE to TM polarized emission has been observed at a wavelength of ~ 240 nm in good agreement to simulations based on $\mathbf{k} \cdot \mathbf{p}$ -perturbation theory.

HL 33.11 Wed 17:30 Poster F

Optical and structural properties of lattice matched AlInN/GaN heterostructures — ●SAVUTJAN SIDIK, PHILIPP HORENBURG, FEDOR ALEXEJ KETZER, PHILIPP HENNING, HEIKO BREMERS, UWE ROSSOW, and ANDREAS HANGLEITER — Institute of Applied Physics, TU Braunschweig, Germany

It is well known that AlInN can be grown lattice-matched on c-plane GaN. In contrast, on non- and semipolar GaN surfaces, one-dimensional lattice matching can be achieved due to different a/c lattice ratios. This opens up new opportunities to manipulate the strain states in the GaInN/GaN quantum well based light emitting diodes which are suffering from strongly reduced efficiencies towards longer wavelength emissions. However, the basic optical properties of AlInN are not yet well known which are of significant importance not only in accurate characterization of the optoelectronic devices but also in evaluation of the structural quality and homogeneity of the samples. In this contribution, we present first results on the optical investigation of lattice matched AlInN heterostructures grown by MOVPE on c-plane, m-plane and semipolar GaN buffer layers grown on various substrates. Photoluminescence spectroscopy is used to characterize the samples with 266 nm laser excitation in the temperature range of 5 K to 300 K. As an initial step, we observe strong polarization-dependent defect related AlInN emission from the sample grown on semipolar orientation at room temperature. An accurate analysis of the strain state of the epitaxial layers by high resolution XRD is combined with the optical characterization.

HL 33.12 Wed 17:30 Poster F

Structural and opto-electrical investigation of InGaIn/GaN nanoLED arrays — ●JAN GÜLINK^{1,2}, HENDRIK SPENDE^{1,2}, HUTOMO SURYO WASISTO^{1,2}, and ANDREAS WAAG^{1,2} — ¹Institute of Semiconductor Technology (IHT), Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany — ²Laboratory for Emerging Nanometrology (LENA), Technische Universität Braunschweig, Langer Kamp 6a, D-38106 Braunschweig, Germany

In recent years, gallium nitride-based LEDs have been continuously developed and employed in not only solid state lighting but also for bio-imaging and optical sensor applications. By integrating them with CMOS control electronics, matrix-addressed GaN microLED arrays could be utilized as a new microscope technique in life sciences. Although those optoelectronic devices exhibit promising results, their spatial resolution is still low, which results from the LED dimensions

with pixel and pitch sizes in the range of several tens of micrometers.

In this work, InGaN/GaN nanoLED arrays were designed and fabricated to be used as a nanoillumination source inside an on-chip microscope. As the LED pixel dimensions are scaled down to the sub-micron range, the relationship between the nanoscale size and performance of a LED is of interest. Opto-electrical measurements of nanoLEDs were conducted with nanoneedle probing tips inside an SEM. Hence, I-V and electroluminescence characteristics of light sources with dimensions of smaller than one micrometer could be extracted. Technological details of the challenging processing of these structures will also be presented.

HL 33.13 Wed 17:30 Poster F

Dose and bias dependend cathodoluminescence efficiency of InGaN/GaN MQWs — ●HENDRIK SPENDE¹, JOHANNES LEDIG^{1,2}, CHRISTOPH MARGENFELD¹, ANGELINA VOGT¹, SÖNKE FÜNDLING¹, HERGO-HEINRICH WEHMANN¹, TOBIAS VOSS¹, and ANDREAS WAAG¹ — ¹Institute of Semiconductor Technology and Laboratory for Emerging Nanometrology, Braunschweig University of Technology, 38092 Braunschweig — ²Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

Cathodoluminescence (CL) inside a scanning electron microscope (SEM) is a powerful tool to probe optical properties of semiconductor microstructures with high spatial resolution. The primary electron probe is scattered and the generated e-h pairs undergo sample related drift and diffusion. Therefore, the radiative recombination inside the material is spatially inhomogeneous and although resolving local electro-optical properties a quantitative interpretation is difficult.

This work aims at understanding the underlying mechanisms to pave the way for a quantitative interpretation. Dedicated MOVPE grown InGaN/GaN test samples were analyzed by CL at room and LN2 temperatures inside a SEM. Each sample contains MQWs emitting at different wavelengths stacked in growth direction. Thus, spectra taken with different electron beam energies provide depth dependent information on the recombination from different MQWs. We observe unexpected time and temperature dependent changes in the CL emission of the samples which suggest electron beam induced changes in carrier dynamics inside the MQW region which is verified by voltage biased CL.

HL 33.14 Wed 17:30 Poster F

Effect of AlGaIn quantum well barrier composition on electro-optical properties of 270 nm light emitting diodes — ●JAKOB HÖPFNER¹, MARTIN GUTTMANN¹, CHRISTOPH REICH¹, LUCA SULMONI¹, CHRISTIAN KUHN¹, PASCAL RÖDER¹, TIM WERNICKE¹, and MICHAEL KNEISSL^{1,2} — ¹Technische Universität Berlin, Institute of Solid State Physics — ²Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Deep ultraviolet (UV) light emitting diodes (LEDs) with emission wavelengths around 270 nm have a wide range of applications such as water purification, sterilization of medical equipment and gas sensing. By varying the composition of the AlGaIn quantum well barriers (QB), many properties of the LED can be affected: The injection efficiency, the internal quantum efficiency and the light extraction efficiency. To investigate these properties, current and polarization dependent electroluminescence measurements of emission spectrum and output power are performed which are then compared to **k-p** and drift diffusion model calculations. A maximum external quantum efficiency (EQE) was obtained for LEDs with an Al mole fraction of 0.69 in the QB. Furthermore, it was found that the fraction of transverse electric polarized light emission increases and the emission wavelength decreases with increasing Al mole fraction in the QB. This is consistent with **k-p** calculations, attributing the changes of EQE to changes in the transition probabilities. Drift diffusion model calculations are used to investigate the influence of the properties of the heterostructure on the EQE. Finally, it will be discussed how to balance the different effects.

HL 33.15 Wed 17:30 Poster F

Sub 240 nm UVC LEDs featuring low contact resistance V-based electrodes on $n\text{-Al}_{0.9}\text{Ga}_{0.1}\text{N}$ — ●LUCA SULMONI¹, FRANK MEHNKE¹, MARTIN GUTTMANN¹, CHRISTIAN KUHN¹, TIM WERNICKE¹, and MICHAEL KNEISSL^{1,2} — ¹Technische Universität Berlin, Institute of Solid State Physics — ²Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

The design and fabrication of III-nitride-based heterostructures is particularly demanding for deep UV LEDs emitting below 240 nm as the external quantum efficiency drastically decreases with decreasing wavelength. In addition, ohmic contacts to $n\text{-Al}_x\text{Ga}_{1-x}\text{N}$ are extremely challenging for very high Al mole fractions mainly due to the low elec-

tron affinity and to limitations in the ionized donor concentration. This results in high operating voltages and resistive heating.

$\text{Al}_{0.9}\text{Ga}_{0.1}\text{N}:\text{Si}$ layers were grown on low defect density AlN by MOVPE with a specific sheet resistivity of $0.3 \Omega \text{ cm}$. In this study, we achieved ohmic contacts on $n\text{-Al}_{0.8}\text{Ga}_{0.2}\text{N}$ with estimated specific contact resistivities of $9 \cdot 10^{-4} \Omega \text{ cm}^2$. By further optimizing the four-metal electrode V/Al/Ni/Au configuration and the rapid thermal annealing procedure, we were able to sensibly reduce also the contact resistivities as well as the Schottky behavior of our n-contacts on $n\text{-Al}_{0.9}\text{Ga}_{0.1}\text{N}$. The V/Al/Ni/Au n-contacts on $n\text{-Al}_{0.9}\text{Ga}_{0.1}\text{N}$ annealed at 750°C exhibited moderate rectifying characteristics with estimated specific contact resistivities as low as $3 \cdot 10^{-3} \Omega \text{ cm}^2$ at a current density of 0.1 kA/cm^2 . Finally, we fabricated UVC LEDs emitting at 234 nm with output power of $40 \mu\text{W}$ at 20 mA and 12.5 V in cw operation.

HL 33.16 Wed 17:30 Poster F

Instability of the Sb vacancy in GaSb — ●NATALIE SEGERCRANTZ^{1,2}, JONATAN SLOTTE², FILIP TUOMISTO², KENICHIRO MIZOHATA³, and JYRKI RÄISÄNEN³ — ¹Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Germany — ²Department of Applied Physics, Aalto University School of Science, Finland — ³Department of Physics, University of Helsinki, Finland

The narrow-gap semiconductor GaSb can be used in various optoelectronic devices. Undoped, GaSb is of *p*-type and the Ga antisite and the Ga vacancy have been shown to be responsible for the residual hole concentration. Self-diffusion experiments in GaSb have revealed another unusual asymmetry of GaSb. The Ga atom was found to diffuse three orders of magnitude faster in the material than the Sb atom. The Sb vacancy has been proposed to be unstable, exchanging sites with a neighboring Ga atom. This mechanism would enhance Ga diffusion due to the increased Ga vacancy defects while at the same time suppressing Sb diffusion.

We have studied the instability of the Sb vacancy by irradiating undoped, *p*-type GaSb and performing positron annihilation spectroscopy in the temperature interval 35-300 K. The Sb vacancy is shown to be unstable above temperatures of 150 K and undergoes a transition resulting in a Ga vacancy and a Ga antisite leading to a further increase in the acceptor-type defect distribution in proton irradiated material. The activation energy of this transition is determined to be $0.6 \text{ eV} \pm 0.1 \text{ eV}$. Our results prove that the instability of the Sb vacancy in GaSb has a profound role on the native defect distribution in GaSb.

HL 33.17 Wed 17:30 Poster F

Emission and Disorder Properties of Quaternary GaInAsBi Semiconductor Alloys — ●JULIAN VELETAS¹, THILO HEPP², LUKAS NATTERMANN², KERSTIN VOLZ², and SANGAM CHATTERJEE¹ — ¹I. Physikalisches Institut, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany — ²Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, D-35032 Marburg, Germany

Dilute bismuth-containing semiconductor alloys such as Ga(As,Bi) are attracting significant attention due to their promising characteristics in near- and mid-infrared laser applications. The incorporation of bismuth leads to a strong reduction of the bandgap commonly described by an anti-crossing model of the Bi-level with the valence bands of the host material. Consequently, the band gap narrows and the separation Δ_{SO} between the valence band edge and the split-off band increases. If Δ_{SO} surpasses E_{gap} , this leads to a suppression of non-radiative Auger recombination and, thus an enhanced performance of future devices. For example, Δ_{SO} surpasses the bandgap energy E_{gap} for more than 4% bismuth incorporation in (Ga,In)(As,Bi) alloys with In concentrations of about 50%. Here, we study a series of (Ga,In)(As,Bi)/(Ga,In)As/InP epilayers grown by metal-organic vapor-phase epitaxy. Modulation spectroscopy is applied to identify the optical transitions in the quaternary alloy. Comparing the results with temperature-dependent photoluminescence data measurements reveals only a small Stokes Shift and very little disorder signatures.

HL 33.18 Wed 17:30 Poster F

Single Quantum Dot with Microlens and 3D-Printed Microobjective as Integrated Bright Single-Photon Source — ●JAN HAUSEN¹, SARAH FISCHBACH¹, TIMO GISSL², SIMON RISTOK², KSENIA WEBER², SIMON THIELE³, TOBIAS HEINDEL¹, SVEN RODT¹, ALOIS HERKOMMER³, HARALD GIESSEN², and STEPHAN REITZENSTEIN¹ — ¹Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany — ²4th Physics Institute and Research Center SCoPE, Stuttgart, Germany — ³Institute for Applied Optics and Research Center SCoPE, Stuttgart, Germany

In recent years, semiconductor quantum dots (QD) have proven to work as close to ideal single-photon sources. In order to apply such sources in future quantum communication systems, it will be crucial to further increase the photon-extraction efficiency. Here we report on deterministically fabricated QD-microlenses combined with 3D printed microobjectives (MO). Monolithic microlenses were fabricated in a deterministic way by in-situ electron beam lithography allowing for spatial and spectral pre-selection of suitable QDs. Two-photon 3D direct laser writing enabled the realization of multilens MOs precisely aligned to the brightest microlens structures. A micro photoluminescence characterisation of the resulting combination shows an enhancement of the photon-extraction efficiency by a factor of two. The device also exhibits a high suppression of multiphoton events with $g^{(2)}(\tau = 0) < 0.02$.

HL 33.19 Wed 17:30 Poster F

A first-principles investigation of the cubic ternary AlxB1-xBi alloys for infrared optical devices — ●BELABBAS MAWLOUD¹, ARBOUCHE OMAR², BENALLOU YACINE¹, and BENTAYEB ABDELKADER¹ — ¹Laboratory of Technology of Communications, Faculty of Technology, University of Saïda Dr Tahar Moulay, P. O. Box 20000, Saïda, Algeria — ²Laboratory of physico-chemistry of advanced materials, Faculty of Sciences, University of Djillali Liabes, P. O. Box 22000, Sidi Bel Abbes, Algeria

In this study, We propose the cubic AlxB1-xBi ternary alloy as a promising infrared material. we used the full potential-linearized augmented plane wave (FP-LAPW) method within the Density Functional Theory (DFT) to predict the structural, electronic and optical properties of the AlxB1-xBi ternary alloys. The structural properties such as the equilibrium lattice parameter, bulk modulus and its pressure derivative are investigated with the effect of the concentration variation of Al atom, x (x=0, 0.25, 0.50, 0.75 and 1). We found that the equilibrium lattice parameter of AlxB1-xBi ternary alloys increases when increasing the doping concentration of the Al atom, while its bulk modulus decreases. The energy band gap of the AlxB1-xBi ternary alloys decreases with the increase in the Al doping concentration. Our results show the direct nature of the energy band gap of the ternary AlxB1-xBi alloy for all composition of Al substitution. Furthermore, investigation of the dielectric function and refractive index shows that our materials are active in infrared and visible energy regions.

HL 33.20 Wed 17:30 Poster F

Subsecond nuclear spin dynamics in n-doped GaAs — ●PAVEL SOKOLOV^{1,2}, MIKHAIL PETROV², KIRILL KAVOKIN^{2,3}, MARIA KUZNETSOVA², SERGEY VERBIN², DMITRI YAKOVLEV^{1,3}, and MANFRED BAYER^{1,3} — ¹Experimentelle Physik 2, TU Dortmund, Dortmund, Germany — ²Spin Optics Laboratory, Saint Petersburg State University, St. Petersburg, Russia — ³Ioffe Physical Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia

In this work, we report experimental studies of the Nuclear Spin (NS) relaxation in presence of optical excitation in n-doped GaAs ($n_d = 4 \cdot 10^{15}$). The time-resolved photoluminescence study allows us to address a fast subsecond NS dynamics. The NS relaxation time, T_S , is extracted by the time-of-flight method commonly used for investigation the kinetics of the photoluminescence decays. Extrapolation of the subsecond spin relaxation times a weak power of excitation allows us to conclude on the existence of the fast NS relaxation dynamics, which has not been studied so far. We show, that the process is governed by the dynamic polarization of NSs subject to an external magnetic field a time-dependent Knight field of photo-generated electrons encourage also the warm-up of NS bath and relaxation of the non-equilibrium NS. We find that the spin relaxation time T_S is observed in a subsecond time range showing a decrease of T_S from 75 ms down to 40 ms with the pumping power varied by an order of magnitude. The experimental results are interpreted within the developed model predicting a drop of the NS polarization when the light helicity modulation rate reaches a characteristic value determined by ratio $1/\sqrt{T_1 T_2}$.

HL 33.21 Wed 17:30 Poster F

In-situ atomic layer deposition of high-k dielectrics on MBE-grown GaAs — ●SORAYA KARIMZADAH¹, TORSTEN RIEGER¹, NILS VON DEN DRIESCH¹, LIDAI KIBKALO¹, GREGOR MUSSLER^{1,2}, DETLEV GRÜTZMACHER², and MIHAIL ION LEPSA² — ¹Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich GmbH & JARA-FIT, 52425 Jülich — ²Peter Grünberg insitute (PGI-10), Forschungszentrum Jülich GmbH & JARA-FIT, 52425 Jülich

The deposition of high-k dielectrics on III-V compound semiconductors by atomic layer deposition (ALD) is a promising approach to fabricate

gate oxides of Nano devices as well as surface passivation of nanowires (NWs). Employing ALD allows for conformal overgrowth of high aspect ratio structures such as NWs. Here, we have investigated the in-situ ALD of Al₂O₃ and HfO₂ on MBE grown GaAs layers. The experiments were carried out in a state of the art multi-material cluster tool composed of UHV growth and deposition systems. The quality of the ALD layers was first determined. Later on, the in-situ deposition of Al₂O₃ and HfO₂ on GaAs substrates has performed. The MBE-grown GaAs layers transferred directly to the ALD chamber without exposing the samples to air. In this way, the formation of the native oxide and other contamination on the GaAs surface is avoided improving the quality of the semiconductor interface.

The samples were characterized by Ellipsometry, XRR, AFM, RBS, TEM, and CV measurements. High quality high-k dielectrics on III-V semiconductors open the way to nanoscale devices.

HL 33.22 Wed 17:30 Poster F

LH-HH Splitting in Ga(As,Bi) Semiconductor Alloys — ●FREDERIK OTTO¹, JULIAN VELETAS¹, LUKAS NATTERMANN², KERSTIN VOLZ², and SANGAM CHATTERJEE¹ — ¹Institute of Experimental Physics I, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany — ²Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Hans-Meerwein-Str., D-35032 Marburg, Germany

The dilute bismuthide III-V semiconductors are of great interest for a wide range of applications as they offer significant potential for band gap engineering. The anti-crossings of the isovalent Bi level in the uppermost valence bands of the host material potentially allow for the suppression of non-radiative Auger recombination, thus enhancing radiative output characteristics important for the efficiency of semiconductor lasers. In addition, the incorporation of Bismuth causes a splitting of the heavy-hole (hh) and the light-hole (lh) bands at the Γ -point due to a reduction in tetrahedral symmetry of the zinc-blende structures. We investigate a series of Ga(As,Bi)-samples with varying Bismuth concentration and known strain grown by metal-organic vapor-phase epitaxy. We perform low-temperature photomodulation reflectance spectroscopy in order to get detailed information about the optical properties and to quantify the lifting of the hh-lh degeneracy at the Γ -point.

HL 33.23 Wed 17:30 Poster F

Inverted HEMT structure with electric field induced 2DEG — ●ISMAIL BÖLÜKBASI, JULIAN RITZMANN, ANDREAS D. WIECK, and ARNE LUDWIG — Ruhr-Universität Bochum, D-44780 Bochum, Germany

Two-dimensional-electron gases (2DEG) have interesting physical properties and allow studies in reduced dimensions. For example they can function as a host material for electrostatic qubit systems, like quantum dots. These 2DEGs are mostly created in high-electron-mobility transistors with modulation doping.

However, there are deep donor levels, that hinder compatibility with photonic applications. Approaches like short-period-superlattice doping^[1] lead to unwanted gate hysteresis. All structures seem to be plagued by charge noise, probably arising from the dopands in the modulation doped region. To avoid the interference with the impurities, the 2DEG can alternatively be induced with an electric field.

An issue with these structures is to produce reliable ohmic contacts to the 2DEG without short-circuits to the inducing gate. Here we use an approach with alloyed ohmic contacts to a global backgate, inducing the 2DEG. The 2DEG is then contacted with non-alloyed epitaxial contacts.

[1] Umansky, V., et al. "MBE growth of ultra-low disorder 2DEG with mobility exceeding $35 \cdot 10^6 \text{ cm}^2/\text{Vs}$." *Journal of Crystal Growth* 311.7 (2009): 1658-1661.

HL 33.24 Wed 17:30 Poster F

Formation and characterization of shallow junction in GaAs made by ion implantation and ms-range flash lamp annealing — ●JUANMEI DUAN and MAO WANG — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany

With the demand of aggressive scaling in MOS device the further progress can be realized by integration of high mobility semiconductors with CMOS technology. III-V compound semiconductors are characterized not only by the high carrier mobility but most of them are also direct band gap semiconductors. In this paper we present the formation of shallow junctions in both p-type and n-type GaAs utilizing ion

implantation of S and Zn, respectively, followed by millisecond-range flash lamp annealing (FLA). The distribution of implanted elements obtained by SIMS shows that the FLA process suppressed the diffusion of dopants and simultaneously the ms-range annealing is sufficient to recrystallize the implanted layer. The effective carrier concentration is in the range of $5 \times 10^{18} \text{ cm}^{-3}$ suggesting full activation of implanted elements. Formation of p-n and n-p junction is confirmed by current-voltage characteristics and photoluminescence spectroscopy where the main emission peak from the implanted GaAs layer exhibits red and blue shift, respectively. The observed shift is due to the Burstein-Moss-Effect. Moreover, the Raman active LO-like phonon mode in Zn doped GaAs exhibits a strong asymmetry on the left side due to a coupling with the plasmon mode. This is typical for p-type GaAs with a carrier concentration higher than 10^{18} cm^{-3} .

HL 33.25 Wed 17:30 Poster F

Rotational twins in III-V/Si(111) virtual substrates and their impact on subsequent III-V nanowire growth —

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The epitaxial integration of III-V nanowires (NWs) with Si combines the tunable, high-performance properties of III-V materials with the well-established Si technology. In particular the combination of (111) oriented epilayers/transition layers with the vapor-liquid-solid (VLS) growth of doped, NW-based III-V structures is a subject of intense research. However, the epitaxy on (111) orientation is generally accompanied by the formation of rotational twins. In the present study, we thoroughly investigate the twin suppression in GaP/Si(111) virtual substrates below 5 vol%. In particular, the misorientation of the vicinal Si substrate has a crucial influence on the resulting twin density. We explain the underlying mechanism by a DFT and KMC based nucleation model and show the impact of rotational twin boundaries (RTBs) in GaP/Si on the subsequent NW growth both for GaP and GaAs NWs. RTBs can suppress NW growth entirely or lead to different undesired growth directions, such as horizontal and diagonal growth. To explain the similarities and differences of GaP and GaAs NW growth, we developed a second model based on classical nucleation theory.

HL 33.26 Wed 17:30 Poster F

A series of "fractional" peaks in multiple paramagnetic resonance Raman scattering by (Cd,Mn)Te quantum wells — ALEXEI KOUDINOV^{1,2}, ALEXANDER KNAPP³, GRZEGORZ KARCZEWSKI⁴, •SEBASTIAN ELSÄSSER³, and JEAN GEURTS³ — ¹Spin Optics Laboratory, St.-Petersburg State University, St.-Petersburg, Russia — ²A.F. Ioffe Physico-Technical Institute of RAS, Russia — ³Physikalisches Institut (EP3), Universität Würzburg, Germany — ⁴Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Diluted magnetic semiconductors (DMS) are employed as a ground for the analysis of spin interactions between the band charge-carriers and the localized spin moments of magnetic ions. In 1995, multiple paramagnetic resonance (MPR) Raman scattering was discovered in narrow QWs of the (Cd,Mn,Mg)Te family: a large number of equidistant Raman repetitions, with energy shifts being integer multiples of the Zeeman splitting of the intra-shell Mn 3d₅ electrons. We report on a previously unknown series of B-field dependent Raman lines in MPR conditions in a model DMS QW nanostructure. The observed series of lines shows up in the gaps between the main MPR peaks in a narrow range of B-fields (around 6 T) and seems to manifest a fractional effect: a spin flip of a half-integer number of Mn 3d₅ electrons. The peaks reveal remarkably weak dependence of the intensity on the peak number. We demonstrate some main peculiarities of the observed series of lines, discuss the appropriateness of the fractional- as well as alternative interpretations and we discuss steps towards a further exploration of the effect.

HL 33.27 Wed 17:30 Poster F

Optical and magnetic studies of MBE-grown ferromagnetic CrSe and CrS layers in zincblende structure — •JOHANNES RÖDER¹, RICHARD T MOUG², KEVIN A PRIOR², and WOLFRAM HEIMBRODT¹ — ¹Department of Physics and Material Science Center, Philipps University, Marburg, Germany — ²Institute of Photonics and Quantum Sciences, SUPA, School of Engineering and Physical

Sciences Heriot-Watt University, Edinburgh, United Kingdom

Theoretical calculations predicted chromium chalcogenides in the zinc blende (ZB) structure to be promising candidates for half-metallic spin-aligner at room temperature. Unfortunately, the thermodynamically stable phase of CrSe and CrS is the hexagonal NiAs-structure. Different approaches have been tested to stabilize the ZB state. Most promising were CrSe layers grown on GaAs substrates with either ZnSe or ZnSe/MgS as buffer layers and CrS-layers embedded between Zn-MgS layers. All samples have been grown by MBE. We investigated the ferromagnetic properties and magnetic phase transitions and the respective optical properties of these films by temperature dependent SQUID and time resolved photoluminescence measurements. Ferromagnetic phase transitions have been found. The highest yet observed Curie temperature was at 255 K. Optical measurements revealed excitonic transitions of ZnSe, CrSe as well as the type-II CrSe-ZnSe inter-layer transition.

HL 33.28 Wed 17:30 Poster F

Towards electrostatically defined Quantum Dots in ZnSe —

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ZnSe is a promising material for realizing electrostatically defined electron spin qubits combining both long coherence and optical activity. Unlike the current materials (Ga,Al)As and SiGe, our ZnSe/(Zn,Mg)Se quantum wells exhibit neither valley splitting nor a nuclear magnetic field if isotopically purified combining their strengths. As the effective mass of ZnSe is three times higher compared to GaAs, small gate patterns are required for single electron trapping.

Therefore, we demonstrate lift-off gate pattern for double quantum dots with feature size of less than 20 nm on Si substrates, which are sufficient for our ZnSe/(Zn,Mg)Se heterostructure according to simulations. In order to avoid electrical noise from doping, we implant dopants below ohmic contacts and heal/activate them by annealing. Heating ZnSe appears to be problematic due to the loss of Zn, which compensates our n-doping. Therefore, we present our studies on annealing in a Zn atmosphere using different implantation energies and species.

HL 33.29 Wed 17:30 Poster F

Optical spectroscopy on single semiconducting hetero dot-in-rod nanostructures: A comparison of type-I (CdSe/CdS) and type-II (ZnSe/CdS) systems — •HANS WERNERS, SVEN LOHMANN, ALEXANDRA HINSCH, CHRISTIAN STRELOW, TOBIAS KIPP, and ALF MEWS — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Single CdSe/CdS dot-in-rod nanostructures are well researched in terms of their optical properties. The band offset of these structures characterizes CdSe/CdS as Type-I semiconductors. Here, we compare recent results obtained in single-nanocrystal spectroscopy of CdSe/CdS dot-in-rods [1] to results on type-II systems.

For this approach we successfully synthesized ZnSe/CdS dot-in-rods. Single ZnSe/CdS dot-in-rod structures were investigated by confocal fluorescence spectroscopy at room and cryogenic temperatures. We measured lifetimes, intensity time traces, emission spectra, and polarization properties of these dot-in-rods for different excitation wavelengths. Our first data indicate a type-II behavior leading to considerably longer lifetimes as compared to the CdSe/CdS case.

[1] S. Lohmann et al., ACS Nano Article ASAP DOI: 10.1021/acsnano.7b05303

HL 33.30 Wed 17:30 Poster F

Transparent UV-active solar cells based on NiO/ZnO heterostructures: Suppression of interface recombination currents — •ROBERT KARSTHOF, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, Linnéstraße 5, 04103 Leipzig, Germany

Visible-light-transparent photovoltaic cells open new fields of application for solar cells, such as energy harvesting on windows, glass roofs or displays of mobile devices. It has been shown [1] that p-NiO/n-ZnO heterojunctions show photovoltaic activity in the UV spectral range. They suffer, however, from a severe illumination-induced increase of the carrier recombination rate at the type-II heterointerface. Because

of the strong offsets in valence and conduction bands of the heterostructure, recombination through interface gap states is the dominating transport mechanism under both dark and illuminated conditions.

In this work, we studied the effect of the inclusion of a few-nm-thin insulating layer of HfO_2 between NiO and ZnO , aiming at a suppressed interface recombination by widening the interface gap and reducing the density of states within it. At the same time, it should allow an unhindered transport of photogenerated carriers across.

NiO and ZnO layers were grown by pulsed laser deposition, the HfO_2 buffer layers were deposited by RF sputtering. Device characterization was done by current-voltage, capacitance-voltage and quantum efficiency measurements as well as carrier collection analysis.

[1] R. KARSTHOF, H. VON WENCKSTERN, M. GRUNDMANN: *J. Vac. Sci. Technol. B* **34**, 04J107 (2016)

HL 33.31 Wed 17:30 Poster F

Towards transparent and flexible photovoltaic devices: optimized growth parameters of NiO/ZnO -based UV solar cells in superstrate configuration — ●FABIAN SCHÖPPACH, ROBERT KARSTHOF, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnestraße 5, 04103 Leipzig, Germany

Visible-light transparent solar cells open new areas for photovoltaic energy harvesting, such as on windows, glass roofs or displays of mobile devices. In the work of KARSTHOF et al. [1], ZnO/NiO heterojunctions were used as prototypes of transparent UV active solar cells. The transparency of these cells is mostly limited by the electrode deposited on top of the p -type NiO contact. Thin metallic layers are usually employed for this purpose.

In this work we present an approach to tackle this by replacing the hitherto used ohmic contact with a tunnel junction between the p -type NiO and a TCO electrode, namely indium tin oxide (ITO). Additionally, the overall structure shall be changed to a superstrate configuration to circumvent the necessity of encapsulation. Moreover, flexible instead of rigid glass substrates were used in order to test for the portability into a roll-to-roll fabrication process. p -type NiO and n -type ZnO were grown on ITO-coated flexible glass substrates by pulsed laser deposition. The cells were characterized by means of optical transparency, X-ray diffraction and both, dark and illuminated current-voltage measurements.

[1] KARSTHOF et al. *physica status solidi (a)*, 213.1 (2016): 30–37

HL 33.32 Wed 17:30 Poster F

CVD-growth and characterization of crystalline zinc oxide layers and nanowires — ●FLORIAN HUBER, ANOUK PUCHINGER, WALEED AHMAD, MANFRED MADEL, SEBASTIAN BAUER, RAPHAEL MÜLLER, and KLAUS THONKE — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

For the growth of zinc oxide (ZnO) by chemical vapor deposition (CVD), the commonly used graphite powder as reducing agent is replaced by the gaseous precursor methane (CH_4). By this, the controllability of the growth processes can be significantly improved. Specifically the consumption of the source material (a commercially available ZnO powder) and the II-VI ratio can be varied very precisely.

Using this new growth method, high quality ZnO layers have been grown both on gallium nitride (GaN) substrates and on c -plane sapphire with an intermediate aluminum nitride (AlN) nucleation layer. By adjusting the growth conditions accordingly, it is possible to switch from layer growth to catalyst-free growth of ZnO nanowires on a -plane and c -plane sapphire. The excellent quality of the resulting material is proven by high resolution X-ray diffraction (HRXRD) measurements and low-temperature photoluminescence (PL) spectroscopy.

With the presented method high growth rates can be realized, while keeping the technical setup as simple as possible. Together with the high controllability and the low-cost precursors used, the method has great potential for industrial up-scaling.

HL 33.33 Wed 17:30 Poster F

Optical Characterization of iron-doped ZnO — ●SEBASTIAN BAUER¹, FLORIAN HUBER¹, BENJAMIN NEUSCHL¹, MATTHIAS SCHRECK², and KLAUS THONKE¹ — ¹Institute of Quantum Matter, Semiconductor Physics Group, University Ulm, Germany — ²Institute of Physics, University Augsburg, Germany

Iron is a pertinent impurity even in high-quality II-VI-semiconductor materials. In ZnO , iron on a Zn lattice site acts as a deep donor and can not be used to compensate excess carriers. However, ZnO:Fe is an interesting candidate for the realization of ferromagnetic semiconduc-

tors for spintronics applications.

In this study we present results on the preparation of iron containing ZnO layers grown by chemical vapour deposition. Iron has been incorporated into high-quality crystalline wurtzite ZnO layers both by ion implantation and by a CVD-based seed growth technique adding iron(II) acetate as a precursor. Optical Raman spectroscopy, photoluminescence, and magneto-optical photoluminescence investigations on the iron atom and its optical band at 1.78 eV are presented. This band emerges for Fe^{3+} from the spin-forbidden electric-dipole transition from the excited state ${}^4T_1(G)$ to the ground state ${}^6A_1(S)$ transition.

HL 33.34 Wed 17:30 Poster F

Raman spectroscopy of the copper oxide phases Cu_4O_3 and CuO : A first principles study — MARCEL GIAR, MARKUS HEINEMANN, and ●CHRISTIAN HEILIGER — Institute of Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

We present first principles Raman spectroscopic investigations of the binary oxides Cu_4O_3 and CuO . For monoclinic CuO different (magnetic) unit cells must be considered at room temperature and below 213 K. These structures particularly differ by their local symmetry. The resulting effects on the Raman spectrum are discussed in detail and experimental observations [1] are explained. We further study the laser energy dependence of the Raman spectrum of both the room temperature and the low temperature structure. For tetragonal Cu_4O_3 experimental Raman spectra have only recently been obtained [2,3]. For this material we present a detailed analysis of the Raman scattering properties with particular emphasis on the crystal orientation and the angular dependence of the Raman intensities.

[1] X. K. Chen, J. C. Irwin, and J. P. Franck, *Phys. Rev. B* **52**, R13130 (1995)

[2] B. K. Meyer, A. Polity, D. Reppin, M. Becker, P. Hering, P. J. Klar, T. Sander, C. Reindl, J. Benz, M. Eickhoff, C. Heiliger, M. Heineemann, J. Bläsing, A. Krost, S. Shokovets, C. Müller, and C. Ronning, *Phys. Status Solidi B* **249**, 1487 (2012)

[3] L. Debbichi, M. C. M. de Lucas, J. F. Pierson, and P. Krüger, *J. Phys. Chem. C* **116**, 10232 (2012)

HL 33.35 Wed 17:30 Poster F

H_2S -sensing in the sub-ppm region with a ZnO nanowire ChemFET — ●ANGELIKA KAISER, FLORIAN HUBER, YUJIA LIU, KLAUS KOLB, MANFRED MADEL, and KLAUS THONKE — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

The medical role of hydrogen sulfide (H_2S) has been extensively studied over the past few years, revealing a variety of crucial medical applications. These are reaching from cancer therapeutics to medical diagnostics via breath analysis. Such a reliable breath analysis, which is selectively aiming at the detection of ppb-range concentrations of the biomarker H_2S , requires a gas sensing device with a well understood and effective sensing mechanism.

We investigated resistive gas sensors based on the conductivity change of ZnO NWs under different gas exposure, which effectively act as ChemFETs with open gate. The sensitive element is formed by the surface of ZnO NWs, and operates as a transducer between ongoing adsorption reaction on the NW sensor surface and the resistivity change in the NWs leading to a measurable electrical signal. The goal of our work is to design a stable sensor with an optimal translation of the chemical surface reactions into a detectable electrical signal. Therefore, we grew and electrically compared various sets of VLS grown ZnO NWs, which additionally were characterized by SEM micrographs and analysed by low-temperature PL-spectroscopy.

HL 33.36 Wed 17:30 Poster F

Molecular Dynamics Simulation of the Oxidation Process of thin Silicon Nanowires — ●GEORG HEINZE^{1,2}, FLORIAN FUCHS^{1,2,3,4}, SIBYLLE GEMMING^{2,3,4}, and JÖRG SCHUSTER^{2,4} — ¹Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — ²Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — ³Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — ⁴Center for Advancing Electronics Dresden (cfaed), Dresden, Germany

Silicon nanowires (SiNWs) are promising building blocks for the development of small nanoelectronic devices, such as ultra-scaled field-effect transistors or sensors. The oxidation of the wires has a large impact on their electronic properties. With shrinking device sizes an atomistic modelling of the oxidation process has become increasingly important.

Using molecular dynamics with a reactive force field potential we analyse the beginning of the oxidation process of thin SiNWs. Wires of varying diameters with the orientations $\langle 100 \rangle$ and $\langle 110 \rangle$ are examined regarding the speed of the oxidation at different temperatures. We will show how the mass density, the stoichiometry and the mechanical strain evolve during the oxidation process. The observation of multiple different subphases during the oxidation is one exemplary finding.

HL 33.37 Wed 17:30 Poster F

Irradiation Effects on β -Ga₂O₃ Single Crystal: Vacancy vs. Optical Properties — •CHAOMING LIU¹, YIDAN WEI¹, MAO WANG^{2,3}, YONDER BERENCÉN², JIANQUN YANG¹, XINGJI LI¹, and SHENGQIANG ZHOU² — ¹Harbin Institute of Technology, School of Materials Science and Engineering, 150001, Harbin, China — ²Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, D-01328, Dresden, Germany — ³Technische Universität Dresden, D-01062, Dresden, Germany

Monoclinic beta-phase gallium oxide (β -Ga₂O₃) is a versatile transparent conducting oxide with excellent chemical and thermal stability and a wide bandgap of 4.85 eV. In β -Ga₂O₃, vacancies play a crucial role, largely influencing the optical properties. However, the optical response induced by vacancy-engineering in β -Ga₂O₃ has so far been only investigated under quasi-stationary conditions. Therefore, the research on the dynamic correlation between the optical properties and vacancies of β -Ga₂O₃ is of great interests. In this work, n-type β -Ga₂O₃ single crystals are irradiated by 25 MeV O ions with different fluences to investigate the effect of vacancies. The correlation between the vacancy concentration and the optical properties is investigated

by Raman spectra and photoluminescence experiments. We show that the symmetric stretching modes and bending vibrations of GaO₄ and GaO₆ units are weakened to a certain extent upon increasing irradiation fluence. Moreover, the emission at the blue and green regions is enhanced upon raising the vacancy density, while the UV emission is strongly reduced.

HL 33.38 Wed 17:30 Poster F

The Effect of Oxygen Vacancies on the Creation and Migration of Ti Interstitials in r-TiO₂ — •JULIAN GABERLE and ALEXANDER SHLUGER — University College London, WC1E 6BT London, UK

Titanium dioxide finds a wide range of applications from catalysis, electronics, gas sensing to paint. Its broad range of uses is due to its exceptional physical properties i.a. high refractive index, high dielectric and hardness. In its stoichiometric form TiO₂ is a wide bandgap insulator. However, defects and impurities can create states, which lie in the bandgap, thus altering its physical properties. Understanding these defect states is imperative to building new technologies and other future applications.

The two most important defects in TiO₂ are oxygen vacancies and titanium interstitials. Both defects create a defect state just below the conduction band. This defect state is commonly attributed to the formation of polarons on titanium sites, creating a Ti³⁺ species.

In this work, we used ab initio methods to investigate the interplay between oxygen vacancies and Ti interstitials. It was found that the barrier for Frenkel defect formation is significantly reduced in the presence of O vacancies. Furthermore the diffusion barrier of Ti interstitials is dependent on the degree of reduction.