

## HL 36: Poster III

Time: Wednesday 16:30–19:00

Location: Poster D

HL 36.1 Wed 16:30 Poster D

**Theory of the low temperature phase of succinonitrile** — ●IMAD BELABBAS, JOHAN CARLSSON, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck Gesellschaft, Faradayweg 4-6, D-14 195 Berlin-Dahlem (Germany)

Recently, succinonitrile has emerged as a promising solid electrolyte for lithium batteries [1]. Succinonitrile is a molecular crystal that crystallizes into two different phases. Below 233 K, succinonitrile has a perfectly ordered structure that only contains gauche isomers. Between, 233 K and 331 K, succinonitrile is a plastic crystal that contains a mixture of molecules with gauche and trans conformations. As a first step toward studying the full properties of succinonitrile, we have investigated the crystal structure of the low temperature phase. For the latter, only the lattice parameters are known, but not the position of the molecules in the unit cell. We have adopted a two steps approach, where force field and density-functional theory (DFT) calculations were applied. Initially, an extended scan of the configurational space was performed where the structures were ordered according to their non-bonded molecular interaction energy. This provided a set of potential candidates that were used as input for a global minimum energy search procedure based on genetic algorithms. The obtained configuration of the unit cell was further refined by means of DFT calculations. This procedure led to a theoretical structural model for the low temperature phase of succinonitrile.

[1]- J. P. Alarco, Y. Abu-Lebdeh, A. Abouimrane and M. Armand, *Nature Materials*, 3, 476 (2004).

HL 36.2 Wed 16:30 Poster D

**Determination of electrochemical potentials of organic semiconductors via cyclic voltammetry and their relevance for organic photovoltaic devices** — ●CLEMENS FESER<sup>1</sup>, CARSTEN DAIBEL<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg — <sup>2</sup>Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg

An important key parameter of organic bulk heterojunction solar cells is the open circuit voltage (VOC), which maximum is predominantly determined by the energy gap between the HOMO-level of the electron donor and the LUMO-level of the acceptor material. These electrochemical potentials (ECP) can be determined via cyclic voltammetry (CV). The ECP-values sensitively depend on the sample's state of aggregation (solid/liquid), variation of the solution and/or the electrolyte as well as on the choice of the conduction salt. A home-built CV-technique has been set up and was modified to evaluate the optimal conditions for accurate determination of the ECPs of a series of organic semiconductors, e.g. electron donors and acceptors like conjugated polymers and fullerenes, respectively. Further, we prepared organic bulk heterojunction solar cells based on different semiconductor combinations and evaluate the experimentally determined VOC in respect of the electrochemically determined HOMO- and LUMO-energies.

HL 36.3 Wed 16:30 Poster D

**Charge carrier injection studies into wide band gap organic semiconductors** — ●MAXIMILIAN NOTHAFT, FEDOR JELEZKO, JENS PFLAUM, and JÖRG WRACHTRUP — 3. Phys. Ins., Univ. Stuttgart, 70550 Stuttgart, Germany

Charge carrier injection into the LUMO of wide band-gap organic single crystals of small molecules, like naphthalene or anthracene, is difficult to realize because of the request for air-stable contact materials providing low work functions in the range of 2.0eV. E.g. to explore the transport in these molecular semiconductors by FET or SCLC measurements, a stable carrier injection at the respective contact interfaces has to be guaranteed. In this contribution we will present two different approaches on the injection of charge carriers into crystals of the organic semiconductors p-terphenyl and anthracene. At first, free electron injection was performed via a scanning electron microscope at voltages between 5kV to 30kV and, at second, by use of evaporated Al/Au contacts. From space charge limited current measurements up to 200V, we conclude on the transport parameters in these materials. Furthermore, it will be shown that simultaneous injection of holes and

electrons yields to recombination electroluminescence from the wide band-gap host crystals, which resembles that of the optically excited fluorescence spectra. As an outlook, the effect of intentional doping of these organic crystals by certain guest molecules such as pentacene and dibenzoterrylene will be discussed.

HL 36.4 Wed 16:30 Poster D

**Electronic Structure and Charge Transport in Durene Crystals** — ●CHRISTOPH ARNDT<sup>1</sup>, FRANK ORTMANN<sup>2</sup>, KARSTEN HANNEWALD<sup>2</sup>, FRIEDHELM BECHSTEDT<sup>2</sup>, and JENS PFLAUM<sup>1</sup> — <sup>1</sup>3. Phys. Institut, Univ. Stuttgart — <sup>2</sup>European Theoretical Spectroscopy Facility and IFTO, Friedrich-Schiller-Univ. Jena

The intrinsic charge-carrier mobility defines an important material parameter and allows an understanding of the microscopic transport processes in organic semiconductors. Durene has shown one of the best transport performances in single crystals with room-temperature mobilities up to 5 cm<sup>2</sup>/Vs [1]. The bandlike transport behavior in combination with the small conjugated pi-electron system makes durene also attractive for theoretical descriptions by ab-initio DFT calculations [2].

In this contribution we present experimental data on the mobility tensor of durene crystals accompanied by a theoretical analysis including the influence of fundamental vibrational modes. Bridgman crystals were grown from purified material and electronically characterized by the time-of-flight technique. To access the anisotropy of the mobility, durene slabs along different crystallographic orientations were prepared and the charge-carrier mobility was determined in the temperature range between 5K and 300K. The measurements showed a significant increase of the hole mobilities towards lower temperatures reaching values as high as 100 cm<sup>2</sup>/Vs.

[1] Z. Burshtein and D.F. Williams, *Phys. Rev. B* **15**, 5769 (1977).

[2] F. Ortmann, K. Hannewald, and F. Bechstedt, *Phys. Rev. B* **75**, 195219 (2007).

HL 36.5 Wed 16:30 Poster D

**Impedance spectroscopy on polymer solar cells** — ●ROLAND RÖSCH<sup>1</sup>, INGO HÖRSELMANN<sup>2</sup>, ANDREI HERASIMOVIC<sup>2</sup>, SUSANNE SCHEINERT<sup>2</sup>, GERHARD GOBSCH<sup>1</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>Institute of Physics, Ilmenau University of Technology, Weimarer Straße 32, 98693 Ilmenau, Germany — <sup>2</sup>Institute of Solid State Electronics, Ilmenau University of Technology, Gustav-Kirchhoff-Str. 1, 98693 Ilmenau, Germany

Impedance spectroscopy is a powerful tool to investigate internal electrical properties of an electronic device. We use this non-invasive technique to study polymer solar cells based on P3HT:PCBM blends and measure the admittance in dependence on the frequency of the applied voltage and fit the results with an equivalent circuit (EC). The elements of the EC reflect the internal electrical properties as contact behaviour, dielectric constants, depletion layers or charge transport. We varied the hole- and electron extracting contacts by modification layers or different metals. The different interlayers show an influence on charge transport and contact behaviour, which results in different device properties.

HL 36.6 Wed 16:30 Poster D

**Electron spin resonance studies of sol-gel-processed anatase-TiO<sub>2</sub>-nanocrystals and charge transfer in blends with P3HT** — ●ANDREAS SPERLICH<sup>1</sup>, JAN FRIEDMAN<sup>1,2</sup>, INGO RIEDEL<sup>1,2</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — <sup>2</sup>ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg

Light-induced electron spin resonance (L)ESR studies of photogenerated charge carriers in mesoporous films of TiO<sub>2</sub> blended with poly(3-hexylthiophene) (P3HT) were performed. The TiO<sub>2</sub>-films were produced by sol-gel processes. XRD-measurements confirm anatase-structure. In pure films of TiO<sub>2</sub>, several distinct lines are observed under illumination. These excited states are known as "photodoping" and lead to enhanced electrical conductivity. With ESR, they can be assigned to Ti<sub>3</sub><sup>+</sup> and O<sub>2</sub><sup>-</sup> crystal and surface states which form paramagnetic electron and hole traps. Blended with P3HT the spectrum is dominated by one symmetrical line that originates from polarons

on the polymer backbone. With different illumination conditions (UV vs. white light) it can be shown that both, electron transfer from the polymer to the TiO<sub>2</sub> and hole transfer in the other direction, are possible processes for the generation of free charge carriers. The charge transfer efficiency is important for applications in organic-inorganic hybrid solar cells.

HL 36.7 Wed 16:30 Poster D

**Transport Gap and exciton binding energy determination in organic semiconductors** — ●STEFAN KRAUSE<sup>1</sup>, BENEDETTA CASU<sup>2</sup>, ACHIM SCHÖLL<sup>1</sup>, FRIEDRICH REINERT<sup>1</sup>, and EBERHARD UMBACH<sup>1</sup> — <sup>1</sup>University of Würzburg, Experimental Physics II, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Inst. f. Physik. u. Theor. Chemie, Auf der Morgenstelle 8, 72076 Tübingen, Germany

The transport gap of an organic semiconductor is defined as the energy difference between the HOMO and LUMO levels in the presence of a hole or electron, respectively, after relaxation has occurred. Its knowledge is mandatory for the optimisation of electronic devices based on these materials. UV photoelectron spectroscopy (UPS) and inverse photoelectron spectroscopy (IPES) are routinely applied to measure these molecular levels. However, the precise determination of the transport gap on the basis of the respective data is not an easy task. It involves fundamental questions about the properties of organic molecules and their condensates, about their reaction on the experimental probe, and on the evaluation of the spectroscopic data. In particular electronic relaxation processes, which occur on the time scale of the photo excitation, have to be considered adequately. We determined the transport gap for the organic semiconductors PTCDA, Alq<sub>3</sub>, DIP, CuPc, and PBI-H4. After careful data analysis and comparison to the respective values for the optical gap we obtain values for the exciton binding energies between 0.1 - 0.5 eV. This is considerably smaller than commonly believed and indicates a significant delocalisation of the excitonic charge over various molecular units.

HL 36.8 Wed 16:30 Poster D

**Characterization of organic photovoltaic cells in comparison with analytic simulations** — ●CHRISTIAN KÖRNER<sup>1,2</sup>, FLORIAN HOLCH<sup>2</sup>, ACHIM SCHÖLL<sup>2</sup>, CARSTEN DEIBEL<sup>1</sup>, FRIEDRICH REINERT<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VI, 97074 Würzburg — <sup>2</sup>Universität Würzburg, Experimentelle Physik II, 97074 Würzburg

Electronic devices based on organic semiconductors receive a growing interest in fundamental and application related research. One reason is that organic thin film photovoltaic cells promise to offer a cost- and resource-efficient fabrication. In order to achieve higher efficiencies it is indispensable to better understand the fundamental processes within the solar cell and at the interfaces, such as charge-carrier generation, separation and transport.

The samples, composed of Copper-Phthalocyanine (CuPc) and C<sub>60</sub> layers and sandwiched between an ITO-coated glass substrate and metal electrodes, are prepared via organic molecular beam deposition under clean and well defined conditions in ultra high vacuum. By *in-situ* measurements of the current-voltage characteristics, the influence of incident light power, temperature, and cathode material can be investigated in detail.

The experimental results will be discussed in comparison to an analytical simulation of the open-circuit voltage, in view of different models for the charge carrier injection at the electrodes.

HL 36.9 Wed 16:30 Poster D

**Investigation of electronic traps in disordered organic semiconductors via thermally stimulated current measurements** — ●JULIA SCHAFFERHANS, CARSTEN DEIBEL, and VLADIMIR DYAKONOV — Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg

Charge transport in disordered organic semiconductors is generally described as thermally activated hopping in a gaussian distribution of localized states. The presence of charge traps is critical to the performance of organic electronic devices, since trapped charge carriers do no longer contribute to the current flow. The trap distribution in the polymer poly(3-hexylthiophene) (P3HT) is investigated by applying the fractional thermally stimulated current technique. Thereby, a low temperature double-peak distribution has been revealed. One of the peaks is believed to belong to the tail of the intrinsic density of states, whereas the other trap is strongly affected by exposure to oxygen. We discuss the influence of oxygen exposure time on the trap distribution.

HL 36.10 Wed 16:30 Poster D

**Influence of metal structures on the optical properties of organic microcavities** — ●MAIK LANGNER<sup>1</sup>, THOMAS WEIMANN<sup>2</sup>, HARTMUT FRÖB<sup>1</sup>, VADIM G. LYSSENKO<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany, www.iapp.de — <sup>2</sup>Physikalisch-Technische Bundesanstalt AG 2.44, 38116 Braunschweig, Germany, www.ptb.de

Organic semiconductor microcavities combine the advantages of widely tunable light emission with a high gain and comparatively simple processing. For various reasons it is desirable to introduce metal structures into the standard OVCSEL design, e.g. current injection or additional lateral optical structuring due to the high index contrast. We show results of samples containing silver gratings on the micrometer and nanometer scale manufactured by means of shadow mask evaporation and electron beam lithography. They are embedded in a microcavity consisting of two highly reflective SiO<sub>2</sub> / TiO<sub>2</sub> - DBRs and a  $\lambda/2$  -layer of the dye system Alq<sub>3</sub>:DCM. To minimize absorption losses the metal is positioned near to the vertical field minimum at the interface DBR - cavity layer. For the optical investigations we use a microscope setup coupled to a spectrometer which allows for a sub-micron resolution. Changes of the optical properties are compared to FDTD simulations of the electric field distribution.

HL 36.11 Wed 16:30 Poster D

**Monte Carlo simulated charge carrier transport in disordered semiconducting organic devices** — ●JENS LORRMANN<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg — <sup>2</sup>ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg

The charge carrier transport in disordered organic semiconductors plays an important role in understanding and optimizing the behavior of organic electronic devices. It can be described as thermally activated hopping in a gaussian distribution of localized states and is characterized by the charge carrier mobility. In order to investigate this hopping, kinetic Monte Carlo simulations are very helpful, as they allow to gain insight into charge carrier transport properties in such complex systems.

A Monte Carlo program to simulate the charge carrier mobility in disordered organic semiconductors was implemented, taking into consideration the Coulomb interaction. We discuss the influence of charge carrier density, energetic disorder as well as Coulomb repulsion on the mobility.

HL 36.12 Wed 16:30 Poster D

**Investigations of concentration dependent photoluminescence quenching in a P3HT : PCBM bulk heterojunction** — ●JOHANNES KRANTZ<sup>1</sup>, MORITZ LIEDTKE<sup>1,2</sup>, ANDREAS SPERLICH<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — <sup>2</sup>The Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg

The photoluminescence (PL) quenching effect is a strong indicator for charge or energy transfer in photovoltaic polymer - fullerene bulk heterojunctions solar cells. In order to achieve a high photocurrent, an efficient generation of charge carriers is a necessary prerequisite. We present our investigations on the PL-quenching efficiency in P3HT (poly(3-hexylthiophene)) and PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) blends with respect to the donor - acceptor ratio. In order to verify that charge transfer is the dominant process, we conducted electron spin resonance measurements. For a more detailed understanding of the underlying mechanisms of PL quenching, we discuss our data in view of a model by Arkhipov et al.<sup>1</sup> as well as a volume-based model.

HL 36.13 Wed 16:30 Poster D

**Micro-Analysis of fullerene crystals in annealed P3HT-PCBM blends** — ●MAIK BÄRENKLAU, GERHARD GOBSCH, and HARALD HOPPE — Institute of Physics, Ilmenau University of Technology, Weimarer Straße 32, 98693 Ilmenau, Germany

We observe micron-sized needles and other structures of the fullerene derivative PCBM in thin film blends with P3HT upon heat treatment using optical microscopy. Depending on the annealing temperature more and more elongated structures are observed. For lower fullerene contents smaller crystallites are grown. Particular grown fullerene

structures and the corresponding structure-property-relationships are discussed in view of solar cell application.

HL 36.14 Wed 16:30 Poster D

**Numerical simulation of organic bulk heterojunction solar cells** — ●ALEXANDER WAGENFAHL<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, ANDREAS BAUMANN<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — <sup>2</sup>The Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg

By implementing a numerical solver for differential equations, we are able to calculate the current-voltage characteristics of organic bulk heterojunction solar cells. Under illumination, Fermilevel splitting can be observed. By considering different models for polaron dissociation in the active layer as well as charge carrier injection at the interfaces, we are able to compare our simulations to experimental data. In particular, we will discuss the influence of illumination on the solar cell characteristics.

HL 36.15 Wed 16:30 Poster D

**Photophysics of charge transfer in polymer-C<sub>70</sub>-fullerene composites** — ●BJÖRN TITZE<sup>1</sup>, ANDREAS SPERLICH<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, VLADIMIR DYAKONOV<sup>1,2</sup>, and OLEG POLUEKTOV<sup>3</sup> — <sup>1</sup>Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — <sup>2</sup>The Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — <sup>3</sup>Chemistry Division Argonne National Laboratory, 9700 S. Cass Avenue Armonk, IL 60439 USA

Charge polarons in thin films of polymer and polymer-C<sub>70</sub>-fullerene composites are investigated by light induced electron spin resonance at 9.5GHz (X-Band). The materials studied were poly(3-hexylthiophene) (P3HT), [6,6] phenyl-C61-butyric acid methyl ester (PCBM) and a soluble C<sub>70</sub>-derivate. The composites show two distinct polaron signals under illumination and a temperature below 150K, which can be assigned to photogenerated polarons ( $P^+$ ,  $P^-$ ) in the blends. Furthermore, lineshapes and relaxation times have been studied by 130GHz (D-Band) electron spin echo below 30K. The g-tensors of positive polarons ( $P^+$ ) on P3HT and negative polarons ( $P^-$ ) on C<sub>70</sub> have been determined. The T<sub>1</sub>-relaxation time for both spectra is followed by the interaction of the polarons. We discuss the results with regard to applications such as organic bulk heterojunction solar cells.

HL 36.16 Wed 16:30 Poster D

**Characterisation of different hole transport materials as used in organic p-i-n solar cells** — ●STEFFEN PFÜTZNER<sup>1</sup>, ANNETTE PETRICH<sup>1</sup>, CHRISTINE MALBRICH<sup>3</sup>, DIRK HILDEBRANDT<sup>2</sup>, MAIK KOCH<sup>1</sup>, MORITZ RIEDE<sup>1</sup>, KARL LEO<sup>1</sup>, and MARTIN PFEIFFER<sup>2</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany, <http://www.iapp.de> — <sup>2</sup>Heliatek GmbH, Liebigstr. 26, 01187 Dresden, Germany — <sup>3</sup>Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

This work focuses on the replacement of hole transport material MeO-TPD, which has been used so far in organic p-i-n- solar cells despite its has unfavourable behaviour at elevated temperatures. For this reason, different characterisation and investigations of the hole transport materials PV-TPD, PV-TPDoM, Di-NPB and MeO-Spiro-TPD were done, i.e. dopability, hole mobility, absorption, reflection, cyclic voltammetry and glass transition temperature were measured. With simplified structures, e.g. m-i-p diodes, and simplified solar cells, consisting of the blue absorbing fullerene C60 as acceptor and the transparent donor material 4P-TPD, further specific material properties were determined.

HL 36.17 Wed 16:30 Poster D

**Effect of vacuum pressure during metal electrode sublimation on polymer solar cell performance** — ●FLORIAN KÜHNLENZ, GERHARD GOBSCH, and HARALD HOPPE — Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany  
Polymer solar cells based on P3HT/PCBM were prepared identically \* except for a variation in the production parameter of the aluminium electrode sublimation. By increasing the pump-down time of the evaporation chamber the pressure for the aluminium sublimation could be decreased over several decades to different final processing values. We found a clear dependence of the chamber pressure during electrode deposition on the overall solar cell performance. We suggest this pressure dependence to be connected with the slow desorption of O<sub>2</sub> and H<sub>2</sub>O

from the spin cast layers, because the production of the active layer of the solar cell took place at environmental conditions in air and the underlying PEDOT:PSS layer was processed from aqueous solution.

HL 36.18 Wed 16:30 Poster D

**Effect of polymer solar cell geometry on photovoltaic performance** — ●BURHAN MUHSIN<sup>1</sup>, JOACHIM RENZ<sup>1</sup>, KARL-HEINZ DRÜE<sup>2</sup>, GERHARD GOBSCH<sup>1</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — <sup>2</sup>Electronic Technology, Institute of Micro- and Nanotechnologies, Ilmenau University of Technology, Gustav-Kirchhoff-Str. 7, 98693 Ilmenau, Germany

We prepared polymer solar cells using different geometries and active areas to study its effect on energy dissipation during operation. On the one side we have determined experimentally series resistances and performance parameters, on the other side we calculated these values theoretically by making simple assumptions based on the knowledge of solar cell geometry and ITO sheet resistance. Differences occurring between experiment and calculation are discussed. As a result, strategies for optimizing polymer solar cell modules are estimated.

HL 36.19 Wed 16:30 Poster D

**The Local Electronic Structure of planar versus non planar Phthalocyanines (ZnPc, SnPc and PbPc) studied by Resonant Soft X-ray Emission Spectroscopies** — ●NIKOLAOS PELTEKIS<sup>1</sup>, BRENDAN HOLLAND<sup>1</sup>, LOUIS PIPER<sup>2</sup>, ALEX DEMASI<sup>2</sup>, KEVIN SMITH<sup>2</sup>, IG-NATIUS MCGOVERN<sup>1</sup>, and CORMAC MCGUINNESS<sup>1</sup> — <sup>1</sup>School of Physics, Trinity College Dublin, Dublin 2, Ireland. — <sup>2</sup>Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, MA 02215, USA

The electronic structure of thin films of the organic molecular semiconductors: zinc phthalocyanine (ZnPc), tin phthalocyanine (SnPc) and lead phthalocyanine (PbPc) have been investigated by soft x-ray spectroscopy. Near edge x-ray absorption fine structure (NEXAFS) spectra, together with resonant & non-resonant soft x-ray emission (RSXE and SXE) spectra have been measured at the carbon and nitrogen K edges. The resultant spectra measure the unoccupied and occupied carbon and nitrogen 2p projected density of states respectively. In particular, resonant soft x-ray emission spectroscopy results in the site-specific C 2p and N 2p local partial density of states (LPDOS) being measured. An angular dependence of the C 2p and N 2p RSXE spectra of ZnPc, SnPc and PbPc has been observed. The observed angular dependence, the measured LPDOS and their correspondence to the results of density functional calculations will be discussed. Comparison between planar (ZnPc) and non planar (SnPc, PbPc) phthalocyanine along with the differing stacking arrangement of molecules within ZnPc (planar) and SnPc-PbPc (non-planar) crystalline films will be discussed.

HL 36.20 Wed 16:30 Poster D

**Transport in Organic Solar Cells studied with Pulsed Electrically Detected Magnetic Resonance** — JAN BEHREND<sup>1</sup>, ●ALEXANDER SCHNEGG<sup>1</sup>, ELIZABETH A. THOMSEN<sup>2</sup>, IFOR D.W. SAMUEL<sup>2</sup>, DAVID J. KEEBLE<sup>3</sup>, and KLAUS LIPS<sup>1</sup> — <sup>1</sup>Abt. Silizium-Photovoltaik, Hahn-Meitner-Institut Berlin, Berlin, Germany — <sup>2</sup>Organic Semiconductor Centre, School of Physics & Astronomy, University of St Andrews, St Andrews, UK — <sup>3</sup>Carnegie Laboratory of Physics, School of Engineering, Physics, and Mathematics, University of Dundee, Dundee, UK

We report about first pulsed electrically detected magnetic resonance (pEDMR) measurements on organic solar cells at room temperature. Samples containing a blend of MEH-PPV and PCBM were investigated by pEDMR both in spectral as well as in time domain in order to extract information about the electron spin states influencing the current through the device. The pEDMR spectrum gave rise to a single resonance line centered at  $g = 2.0028(5)$  which coincides with a polaron signal recently assigned by continuous wave EDMR. By measuring Rabi oscillations as a function of the spectral position in the pEDMR spectrum, we were able to exploit the unique capabilities of pEDMR to assign current determining spin states not only by their spectral position, but also by their interspin couplings. Plotting the Rabi frequencies as a function of the resonance field, two frequencies could be clearly separated, which resembles the case of two coupled electron spins.

HL 36.21 Wed 16:30 Poster D

**Refined transmission measurement setup for 2D-terahertz**

**photonic crystals** — ●THOMAS KISSINGER and ANDREI PIMENOV — Physikalisches Institut, Universität Würzburg, Germany

We examine transmission spectra of 2D-photonic crystals in the terahertz frequency region quantitatively. We show that the reasons for deviations between calculated (employing FDTD-simulations) and experimental spectra are often not due to sample manufacturing, but due to the optical measuring setup. Issues like high diffraction of terahertz waves, spatial frequency (k-vector) selection of output radiation, deviations from incoming plane-wave illumination and finite size effects of the sample or simulation cell are all important to understand the transmittance of such highly anisotropic objects like photonic crystals. We compare and optimize different experimental and simulation setups in order to obtain stable and mutually consistent results, while keeping the optical system and the models used as simple and straightforward as possible.

HL 36.22 Wed 16:30 Poster D

**Propagation of electromagnetic waves in waveguides based on photonic/plasmonic structures in nanocomposite glass** — ●OLEKSIY KIRIYKO, MORITZ BELEITES, STEFAN WACKEROW, WOLFRAM HERGERT, and HEINRICH GRAENER — Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle

Nanocomposite glass containing metallic nanoparticles is a basis material of plasmonic structures with particular optical properties. Periodic structures are experimentally produced in such a material using an electric field assisted dissolution method. Laser assisted dissolution or modification of nanoparticle containing areas is an elegant way to form waveguides in the twodimensional periodic structures. The finite element method (FEM) implemented in COMSOL/Multiphysics is used to calculate the complex effective permittivity of a two-component material in which equally-sized silver nanoparticles are randomly distributed in a homogeneous dielectric, which is the glass matrix in our case. The properties of different waveguides in triangular lattices in such a nanocomposite glass are investigated. Special attention is devoted to the influence of changes of the geometric structure or of the nanoparticle filling fraction on the waveguide properties. The theoretical investigations are compared with experimental results.

HL 36.23 Wed 16:30 Poster D

**Design of photonic structures: Combination of FDTD methods with genetic algorithms** — ●CHRISTIAN MATYSSEK<sup>1</sup>, STEFAN MEYER<sup>2</sup>, WOLFRAM HERGERT<sup>1</sup>, RÜDIGER WEINER<sup>2</sup>, and MARTIN ARNOLD<sup>2</sup> — <sup>1</sup>Institute of Physics, MLU Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle — <sup>2</sup>Institute of Mathematics, MLU Halle-Wittenberg, Theodor-Lieser-Straße 5, 06120 Halle

The optimal design of properties of photonic crystals and coherent control approaches to light guidance in nanostructures are two application areas where methods to calculate electromagnetic fields in complicated structures have to be combined with optimization methods. To that purpose we construct a compact FDTD algorithm based on a spatial Yee-grid combined with higher-order accurate time integration schemes. In time integration the solver performance is optimized combining an integrator based on well approved Krylov subspace methods (VODPK, ROWMAP) with preconditioning techniques that take into account the specific structure of the model equations. As an effective global optimization method a genetic algorithm is used. As a first example for the application of the method the optimization of band gaps is demonstrated. The application to the optimization of waveguide structures and metallic nanoparticle arrays is discussed.

HL 36.24 Wed 16:30 Poster D

**Thermal emission properties of 2D and 3D Photonic Crystals with and without functionalized surfaces** — ●BENJAMIN GESEMANN, STEFAN L. SCHWEIZER, and RALF B. WEHRSPHON — MLU Halle-Wittenberg, Inst. for physics - AG microMD, Halle, Germany

We present measurements and simulations of the thermal emission properties inside and out of 2D and 3D photonic Crystals using localized integrated emission sources as well as out of plane emission of entirely heated crystals. The photonic crystals were fabricated using a photo-electrochemical etching process allowing us to fabricate deep 2D-structures with aspect ratios (depth/diameter) exceeding 100. By modulating the pore diameter during the etching also 3D-periodic structures can be prepared. Additional functionalized coatings can be used to modify the emission properties and create selective thermal emitter. We will discuss the influence of plasmonic and dielectric

effects on selective thermal emission.

HL 36.25 Wed 16:30 Poster D

**Simulation of light propagation in photonic crystal structures using advanced finite element methods** — ●SVEN BURGER, JAN POMPLUN, FRANK SCHMIDT, and LIN ZSCHIEDRICH — Zuse Institute Berlin, Takustraße 7, D - 14195 Berlin, Germany

Finite element methods allow for accurate and fast simulations of light propagation in micro- and nanostructures. We are developing a programme package for the simulation of time-harmonic light scattering problems and eigenvalue problems based on the finite element method. The package contains higher order finite elements for 1D, 2D and 3D problems, adaptive refinement strategies, and domain decomposition algorithms. We report on the status of the software, and we discuss recent applications of the methods to simulations of photonic crystal fibers [1] and other periodically assembled nanostructures (metamaterials) [2].

[1] G. J. Pearce, G. S. Wiederhecker, C. G. Poulton, S. Burger, and P. St. J. Russell. *Opt. Express* **15**, 12680 (2007).

[2] G. Dolling, M. W. Klein, M. Wegener, A. Schädle, B. Kettner, S. Burger, and S. Linden. *Opt. Express* **15**, 14219 (2007).

HL 36.26 Wed 16:30 Poster D

**Quasiperiodic structures in metallic photonic crystals** — ●CHRISTINA BAUER<sup>1</sup>, DIETMAR NAU<sup>1,2</sup>, SERGEI ZHUKOVSKY<sup>3</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1</sup>4th Physics Institute, University of Stuttgart, 70550 Stuttgart, Germany — <sup>2</sup>Institute of Applied Physics, University of Bonn, 53115 Bonn, Germany — <sup>3</sup>Physics Institute, University of Bonn, 53115 Bonn, Germany

Quasicrystals are aperiodic structures which possess long-range order but no translational symmetry. We fabricated one-dimensional metallic photonic crystals with quasiperiodic lateral spacing. Gold nanowires were arranged on top of an Indium-Tin-Oxide (ITO) waveguide in a Fibonacci sequence or in Cantor sets. Examining the extinction spectra and comparing them to a purely periodic structure, additional peaks arise. The modelling of the extinction spectra both in TE as well as in TM polarization works well using the model of Nau et al. [1], which takes the spatial Fourier transform of the structure together with the waveguide dispersion into account. Angle-dependent measurements also reveal the photonic bandstructure of such quasiperiodic metallic photonic crystal samples.

[1] D. Nau et al., *Phys. Rev. Lett.* **98**, 133902 (2007).

HL 36.27 Wed 16:30 Poster D

**Nonlinear Coordinate Transformation as an Extension of the Fourier Modal Method to Finite-Sized Structures** — ●THOMAS ZEBROWSKI<sup>1</sup>, SABINE ESSIG<sup>1,2,3</sup>, and KURT BUSCH<sup>1,2,3</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe — <sup>2</sup>DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — <sup>3</sup>Karlsruhe School of Optics & Photonics (KSOP), Universität Karlsruhe

The Fourier Modal Method (FMM) can be extended to solve electromagnetic wave propagation problems associated with finite-sized structures. Since the basic algorithm is handling systems which are infinitely periodic in the lateral plane, non-periodic structure simulations via FMM have to introduce an artificial periodicity. In this case, however, interactions between the unit cells are unavoidable unless special measures are taken. Such an isolation of the unit cells may be facilitated through nonlinear conformal mappings. This means that we map the infinitely extended space surrounding the finite-sized structure onto a finite edge layer surrounding the unit cell. The resulting coordinate transformation is easily introduced into the algorithm. On our poster we show that this extended FMM algorithm can treat three-dimensional wave propagation problems that are difficult to solve with other frequency-domain methods such as the finite element approach.

HL 36.28 Wed 16:30 Poster D

**Time-Domain Simulations using Discontinuous Galerkin methods** — ●KAI STANNIGEL<sup>1</sup>, MICHAEL KÖNIG<sup>1,3</sup>, JENS NIEGEMANN<sup>1,2,3</sup>, LASHA TKESHASHVILI<sup>1,2,3</sup>, and KURT BUSCH<sup>1,2,3</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe — <sup>2</sup>DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — <sup>3</sup>Karlsruhe School of Optics & Photonics (KSOP), Universität Karlsruhe

The accurate numerical treatment of complex nano-photonic structures requires a flexible spatial discretization scheme. Standard finite

elements are of limited use for time-domain calculations, since they usually require the inversion of large matrices in each time-step and are thus computationally expensive. This problem can be overcome by the use of Galerkin discontinuous elements. We demonstrate the superior accuracy and performance of this method by applying it to typical problems in the field of nano-photonics. The results are compared to standard methods such as FDTD.

HL 36.29 Wed 16:30 Poster D

**Numerical Treatment of Nonlinearities in Higher-Order Time-Domain Methods** — ●JAN GIESELER<sup>1</sup>, JENS NIEGEMANN<sup>1,2,3</sup>, LASHA TKESHASHVILI<sup>1,2,3</sup>, and KURT BUSCH<sup>1,2,3</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe — <sup>2</sup>DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — <sup>3</sup>Karlsruhe School of Optics & Photonics (KSOP), Universität Karlsruhe

The accurate numerical treatment of field propagation in complex nano-structures often requires the use of higher-order methods. In nonlinear systems, advanced discretization schemes are particularly important to deliver reliable results. In this poster, we demonstrate how to calculate numerical fluxes for the nonlinear Maxwell equations. These fluxes are then used to construct a higher-order discontinuous Galerkin scheme for solving Maxwell's equations with a Kerr nonlinearity. Our approach is further compared to standard methods such as FDTD.

HL 36.30 Wed 16:30 Poster D

**Component Analysis and Optimization of Photonic Crystal Based Semiconductor Laser Diodes** — ●HELMUT ZARSCHIZKY<sup>1</sup>, LIN ZSCHIEDRICH<sup>1,2</sup>, JAN POMPLUN<sup>1,2</sup>, and SVEN BURGER<sup>1,2</sup> — <sup>1</sup>JCMwave GmbH, Haarer Straße 14a, 85640 Putzbrunn, Germany — <sup>2</sup>Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany

Due to the reasonably large photonic bandgap in semiconductor based photonic crystals widely tunable laser diodes seem to be an attractive application. Design and optimization of layer thicknesses, lateral laser channel width, dimension of the unit cell and orientation of the crystal lattice for wave guiding and resonator facets are carried out using FEM-based simulation software. 2D- and 3D-results give detailed suggestions on appropriate resonator designs for wavelength tuning ranges over 100 nanometers in the telecommunication band (1550 nm) and for gas sensing (about 1850 nm).

HL 36.31 Wed 16:30 Poster D

**Defocused Imaging of Fluorescent Beads in Photonic Crystals** — ●SVEN ZIMMERMANN, FRANK CICHOS, and REBECCA WAGNER — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

Photonic crystals are materials with a periodically varying dielectric constant. Multiple scattering of light on this spatially modulated refractive index causes a photonic band structure and photonic band gaps. We show that the fluorescence of emitters embedded into the photonic crystals is spectrally and spatially redistributed. Thus they can be used for studying the angular dependence of the photonic stop band. The photonic crystals are produced by self organisation of polystyrene beads using a vertical deposition technique. A small amount of beads is replaced by dye doped beads. They are detected using defocused fluorescence microscopy. Since the photonic crystal introduces an anisotropy to their emission the defocused imaging patterns are modified compared to a homogeneous medium (which is a medium without band structure). The diffraction patterns show a threefold symmetry which is clearly caused by the photonic crystal since it does not exist for emitters outside of it. This modification of the patterns is compared to simulations of the band structure and defocused images.

HL 36.32 Wed 16:30 Poster D

**Wannier function based numerical analyses of Photonic-Crystal functional elements incorporating optically anisotropic materials** — ●PATRICK MACK<sup>1,2</sup>, DANIEL HERMANN<sup>2,3</sup>, CHRISTOPH KÖLPER<sup>2</sup>, and KURT BUSCH<sup>2,3,4</sup> — <sup>1</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe — <sup>2</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe — <sup>3</sup>DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — <sup>4</sup>Karlsruhe School of Optics & Photonics (KSOP), Universität Karlsruhe

Actively tunable properties of photonic crystals (PCs) may yield the

key to integrated all-optical circuitry, allowing for new devices in optical telecommunication. We present numerical investigations of tunable functional elements in macroporous silicon PC structures based on infiltrating optically anisotropic materials into individual PC pores.

The numerical data has been obtained with the photonic Wannier function approach which is very well suited for computing the optical properties of PC-based optical devices. Recent advances in the experimental realization of such structures indicate that corresponding designs may be realized in the near future.

HL 36.33 Wed 16:30 Poster D

**Chirp dependent Emission of a fs-pumped Semiconductor Disc Laser** — ●ECKHARD KÜHN<sup>1</sup>, ANGELA THRÄNHARDT<sup>1</sup>, STEPHAN W. KOCH<sup>1</sup>, WOLFGANG STOLZ<sup>1</sup>, SANGAM CHATTERJEE<sup>1</sup>, CHRISTOPH LANGE<sup>1</sup>, WOLFGANG RÜHLE<sup>1</sup>, WENDEL WOHLLEBEN<sup>2</sup>, and MARCUS MOTZKUS<sup>3</sup> — <sup>1</sup>Fachbereich Physik, Philipps Universität Marburg, Deutschland — <sup>2</sup>Polymer Research, BASF AG Ludwigshafen, Deutschland — <sup>3</sup>Fachbereich Chemie, Philipps Universität Marburg, Deutschland

We present an experimental study and theoretical analysis of a semiconductor disc-laser system (VCSEL) under coherently controlled, phase sensitive excitation conditions. We show that the sign and the amplitude of the quadratical chirp modifies the total number and the average energy of the injected carriers. This strongly influences the laser gain and therefore the overall VCSEL emission. For the theoretical analysis of this effect, we use nonequilibrium simulations based on the microscopic carrier treatment of coupled Maxwell-multiband semiconductor Bloch Equations. This reveals the physical origin of the experimental findings as the change of the 1s exciton-resonance absorption of the quantum-well barriers due to excitation induced dephasing. The numerical simulations show good qualitative agreement with the experimental data.

HL 36.34 Wed 16:30 Poster D

**Dephasing processes in quantum dot microcavity systems: a microscopic description** — ●SANDRA RITTER, CHRISTOPHER GIES, JAN SEEBECK, JAN WIERSIG, and FRANK JAHNKE — Institut für Theoretische Physik, Universität Bremen

Due to various applications the system of quantum dots placed in three-dimensional optical resonators receives great attention. Starting from a fully quantum mechanical description of the carrier-photon interaction for quantum dots in microcavities, we study the influence of carrier scattering and dephasing on the emission properties. A consistent inclusion of scattering processes in various carrier and photon correlation functions is realized by coupling to acoustic phonons. The interplay of scattering and dephasing is of particular importance in the 'good cavity regime', where the cavity loss rate is smaller than the spontaneous emission rate of the quantum dots into the cavity.

HL 36.35 Wed 16:30 Poster D

**Highly spatial resolved PL spectroscopy of single dislocations in InGaN/GaN quantum well structures** — ●JULIA DANHOF<sup>1</sup>, MATTHIAS EDER<sup>1</sup>, CLEMENS VIERHEILIG<sup>1</sup>, ULRICH T. SCHWARZ<sup>1</sup>, WERNER WEGSCHEIDER<sup>1</sup>, NIKOLAUS GMEINWIESER<sup>2</sup>, ANSGAR LAUBSCH<sup>2</sup>, and BERTHOLD HAHN<sup>2</sup> — <sup>1</sup>NWF II - Physik, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg — <sup>2</sup>Osram Opto Semiconductors, Leibnizstraße 4, 93055 Regensburg

GaN based heterostructures normally show quite high dislocation densities. The impact of the dislocations on the performance of optoelectronic devices is still unclear. With our confocal microscope, we study single threading dislocations for samples with a dislocation density below  $10^7 \text{ cm}^{-2}$ . The impact of threading dislocations on the optical properties of GaN bulk crystals is well known: The dislocations act as nonradiative recombination centers, and the shift of the near band edge emission due to the stress dipole around the dislocation core can be detected by highly spectral resolved photoluminescence (PL) spectroscopy. We now study the impact of single dislocations on the optical properties of InGaN/GaN quantum well structures. By simultaneous detection of the PL signal of both the InGaN quantum well and the GaN barriers, the variation of the quantum well signal can explicitly be attributed to single dislocations which are identified by the GaN emission. The effects in the quantum well are studied in dependency of temperature and excitation density.

HL 36.36 Wed 16:30 Poster D

**Influence of Optical Gain on the Spectral and Temporal Characteristics of 405 nm (Al,In)GaN Laser Diodes Grown on**

**Different Substrates** — ●BERND SCHMIDTKE<sup>1</sup>, TOBIAS MEYER<sup>1</sup>, HARALD BRAUN<sup>1</sup>, ULRICH T. SCHWARZ<sup>1</sup>, DÉSIREE QUEREN<sup>2</sup>, MARC SCHILLGALIES<sup>2</sup>, STEPHAN LUTGEN<sup>2</sup>, and UWE STRAUSS<sup>2</sup> — <sup>1</sup>NWF II - Physik, Universität Regensburg — <sup>2</sup>Osram Opto Semiconductors GmbH

We investigate the spectral and temporal behaviour of violet (Al,In)GaN laser diodes (LDs) emitting at wavelengths of about 405 nm, grown on low dislocation density GaN substrate and on SiC substrate, respectively. LDs on GaN substrate show a broad spectrum with several longitudinal modes above threshold, whereas LDs on SiC substrate partially are lasing on a single longitudinal mode, depending on the driving current. With a high spectral resolution setup we measure the gain below threshold of each longitudinal mode, employing the Hakki-Paoli method. Measurements show a slightly fluctuation of gain for the modes of GaN substrate LDs, but a much higher fluctuation for LDs on SiC substrate. We carry out simulations of the longitudinal mode spectrum of (Al, In)GaN laser diodes using a rate equation model with nonlinear gain effects. Additionally the gain of each longitudinal mode was modified to take the fluctuations of the measured gain into account. With the respective amplitude of these gain fluctuations, the simulated spectra resemble the GaN or SiC substrate LD spectra.

HL 36.37 Wed 16:30 Poster D

**Lateral Mode Behaviour of Broad Ridge 405 nm (Al,In)GaN Laser Diodes: Experiment and Simulation** — ●STEPHAN ROGOWSKY<sup>1</sup>, DOMINIK SCHOLZ<sup>1</sup>, HARALD BRAUN<sup>1</sup>, ULRICH T. SCHWARZ<sup>1</sup>, ANSGAR LAUBSCH<sup>2</sup>, GEORG BRÜDERL<sup>2</sup>, and UWE STRAUSS<sup>2</sup> — <sup>1</sup>NWF II - Physik, Universität Regensburg — <sup>2</sup>Osram Opto Semiconductors GmbH

In the (Al,In)GaN material system lateral ground mode operation of ridge waveguide laser diodes (LDs) is limited to narrow ridge widths up to a few micrometers. For broader ridge LDs, which are inevitable for high output power applications, filaments or higher order lateral modes appear, which influence the far-field beam quality. We investigate the lateral profile of the optical laser mode in the waveguide experimentally and theoretically. We get our experimental results from time resolved scanning near-field optical microscopy (SNOM) measurements on pulsed electrically driven LDs. We measure the number and the width of filaments as a function of ridge width and current density. We compare these experimental data with one-dimensional simulations of the lateral laser mode profile. In these simulations we include the carrier- and thermal-induced modifications of the ridge waveguide refractive index profile. Therefore the spatial resolved rate equations for carriers and photons are solved in a self-consistent loop, including the interaction with the optical mode in the modified refractive index profile. By this method we can simulate the shape of typical measured lateral mode profiles for different ridge widths and current densities with a consistent set of parameters for broad ridge (Al,In)GaN LDs.

HL 36.38 Wed 16:30 Poster D

**Hall effect measurements on AlInN layers with high Indium content and low Hall mobility** — ●KAY-MICHAEL GÜNTHER, HARTMUT WITTE, CHRISTOPH HUMS, ARMIN DADGAR, and ALOIS KROST — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Magdeburg

At AlInN/GaN interfaces grown with strained AlInN on GaN and with Indium concentrations above 32 % a p-channel is expected. For such material, a precise characterization of the electrical and transport properties by Hall-effect measurements is fundamental. In the case of low mobility and/or high resistance such measurements are very difficult: the Hall voltage is about 100-1000 times smaller than the voltage drop without the magnetic field. The apparent Hall coefficient is not caused by a free carrier concentration but rather by dynamic persistent or storage processes due to inhomogeneities within the AlInN layers. However, even in the case of extremely noisy signals useful information, e.g. on the type of carriers can be extracted by comparing the average values of many Hall-effect measurements with and without a magnetic field. Furthermore, the noise can be reduced by lock-in measurements.

HL 36.39 Wed 16:30 Poster D

**Structural and magnetic properties of Eu-, Ho- and Sm-implanted GaN** — ●FANG-YUH LO<sup>1</sup>, VERENA NEY<sup>2</sup>, ANDREAS NEY<sup>2</sup>, ALEXANDER MELNIKOV<sup>1</sup>, DIRK REUTER<sup>1</sup>, SÉBASTIEN PEZZAGNA<sup>3</sup>, and ANDREAS D. WIECK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum — <sup>2</sup>Experimentalphysik, Universität Duisburg-Essen, Lotharstr. 1,

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GaN is a wide band gap semiconductor, which has many applications in high-power electronics as well as optoelectronics. Recently, GaN-based diluted magnetic semiconductors have attracted great interest because theoretical work predicted Curie temperatures above 300K. However, the experimental results are quite different and depend strongly on the fabrication methods. In our studies, the rare-earth elements, Eu, Ho and Sm, are introduced into GaN-based heterostructures by focused ion beam implantation. The structural and magnetic properties of the implanted material are studied.

HL 36.40 Wed 16:30 Poster D

**Near infrared absorption in nonpolar cubic AlN/GaN superlattices** — ●JÖRG SCHÖRMANN<sup>1</sup>, ELENA TSCHUMAK<sup>1</sup>, DONAT J. AS<sup>1</sup>, KLAUS LISCHKA<sup>1</sup>, ERIC A. DECUIR<sup>2</sup>, and OMAR MANASREH<sup>2</sup> — <sup>1</sup>Department of Physics, University of Paderborn, Warburger Str. 100, 33095 Paderborn — <sup>2</sup>Department of Electrical Engineering, University of Arkansas, 3217 Bell Engineering Center, Fayetteville, Arkansas 72701

Nonpolar cubic GaN/AlN superlattices were grown at 720°C by plasma-assisted molecular beam epitaxy on free standing 3C-SiC substrates. 20 periods of AlN/GaN quantum wells were deposited on a 100 nm thick GaN buffer layer. The thickness of the AlN barrier is 1.35 nm for all samples, while the thickness of the GaN well varies between 1.6 nm - 2.10 nm depending on the samples. The periodicity of the GaN/AlN active regions was confirmed by the presence of several peaks in the high resolution x-ray diffraction (HRXRD) spectra. The thickness of the total period was estimated by fitting the HRXRD data using a dynamic scattering theory. Room temperature optical absorption spectra of the intersubband transitions were obtained using a Bruker IFS-125HR spectrometer. Optical absorption was observed in the spectral range of 1.5  $\mu\text{m}$  - 2.0  $\mu\text{m}$  and confirmed theoretically using a square well self-consistent Poisson-Schrödinger model.

HL 36.41 Wed 16:30 Poster D

**Untersuchung von relaxierten und nicht-relaxierten InGaN Quantenfilmen mit Photolumineszenz und Röntgenbeugung** — ●TORSTEN LANGER, HOLGER JÖNEN, LARS HOFFMANN, DANIEL DRÄGER, HEIKO BREMERS, DANIEL FUHRMANN, UWE ROSSOW und ANDREAS HANGLEITER — Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstrasse 2, 38106 Braunschweig

Für optoelektronische Anwendungen im langwelligen Bereich werden InGaN-Quantenfilme mit hohem Indium-Gehalt von grösser 30% benötigt. Da bei so hohem Indium-Gehalt sehr grosse Piezofelder aufgrund der Verspannung zum GaN vorhanden sind, müssen die Schichtdicken fuer eine gute Quanteneffizienz deutlich kleiner als im blau-violetten Bereich sein. Für eine gute Homogenität in der Schichtdicke und der Indium-Konzentration sowie einer guten Injektion der Ladungsträger ist dagegen eine möglichst grosse Schichtdicke vorteilhaft. Für eine Indium-Konzentration von etwa 30% sehen wir eine Relaxation in Röntgenbeugung für Schichten von ca. 2.5nm. Wir stellen vergleichende Messungen von Photolumineszenz und Röntgenbeugung vor zur Frage der Homogenität der Indium-Konzentration an der Schwelle zur Relaxation der InGaN-Quantenfilme.

HL 36.42 Wed 16:30 Poster D

**Oxidation of GaN(0001)-2x2 surfaces by oxygen and water** — ●PIERRE LORENZ, RICHARD GUTT, JUERGEN A. SCHAEFER, and STEFAN KRISCHOK — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Experimental and theoretical studies show a high reactivity of GaN surfaces, which is of importance for various applications [1]. We have performed an in-situ analysis of the interaction of oxygen and water with clean and stoichiometric 2x2 reconstructed GaN(0001) surfaces grown on 6H-SiC(0001) by plasma assisted molecular beam epitaxy, with an RMS roughness well below 1 nm measured by atomic force microscopy. For the as-grown samples, two surface states at 2 eV and 3 eV below  $E_F$  can be found in the ultraviolet photoelectron valence band spectra. Upon oxygen exposure, drastic changes are observed. Within the first 4 Langmuir of oxygen, the state at 2 eV as well as the 2x2 superstructure vanishes. Additionally, the work function  $\phi$  increases by 0.3 eV and a downward bend bending of 0.4 eV is observed. For higher exposures,  $\phi$  remains constant and the valence band spectra merge into curves with two distinct oxygen related states at 6 eV and 11 eV in agreement with earlier works [2,3]. The reaction to water

shows a comparable behaviour, with a disappearance of the 2eV surface state after an exposure of 0.2 L.

[1] C.-L. Hu et al., Chem. Phys. Lett. 424 (2006) 273 [2] V.M. Bermudez, J. Appl. Phys. 80 (1996) 1190 [3] V.M. Bermudez and J.P. Long, Surf. Sci. 450 (2000) 98

HL 36.43 Wed 16:30 Poster D

**Ortsaufgelöste Mikro-EL- und Mikro-PL-Spektroskopie an blauen InGaN/GaN LEDs auf Si(001) und Si(111)** — ●T. FEY<sup>1</sup>, L. REISSMANN<sup>1</sup>, F. SCHULZE<sup>1</sup>, A. DADGAR<sup>1,2</sup>, J. CHRISTEN<sup>1</sup> und A. KROST<sup>1,2</sup> — <sup>1</sup>Institut für Experimentelle Physik, Otto-von-Guericke-Universität, 39016 Magdeburg — <sup>2</sup>AZZURRO Semiconductors AG, Universitätsplatz 2, 39106 Magdeburg

Es wurden MOCVD-gewachsene blaue InGaN/GaN-MQW LEDs auf Si(001)- und Si(111)-Substrat mittels ortsaufgelöster  $\mu$ -EL- und  $\mu$ -PL Spektroskopie untersucht. Die Anregung erfolgte mit der 324 nm Linie eines He-Cd-Lasers, bzw. durch Injektionsströme von bis zu 200 mA. Bei beiden Meßmethoden wurden jeweils die identischen Proben-ausschnitte von 80x200  $\mu$ m<sup>2</sup> abgerastert. Beide Proben zeigen Fabry-Perot-Moden in ihrem Spektrum. Die LED auf Si(001) zeigt eine Blauverschiebung der PL- zur EL-Peakwellenlänge von 15-20 nm. Die Position des Fabry-Perot-Interferenzmusters verschiebt sich mit zunehmenden Strömen im Vergleich zur optischen Anregung. Dies kann nur mit einem veränderten Brechungsindex aufgrund sich ändernder Ladungsträgerdichten erklärt werden. Die einsetzende Rotverschiebung des EL-Peaks deutet auf ein Aufheizen der LED hin. Während die PL-Peakwellenlänge zufällig auf einer lateralen Skala <3  $\mu$ m fluktuiert, treten Domänen von identischen EL-Peakwellenlängen mit 30-50  $\mu$ m Ausdehnung bereits bei Strömen ab 50 mA auf. Offenbar werden lokale Potentialfluktuationen durch die hohe injizierte Ladungsträgerdichte ausgeglichen. Eine auf Si(111) gewachsene Vergleichs-LED zeigt ebenfalls eine blauverschobene PL-Peakwellenlänge.

HL 36.44 Wed 16:30 Poster D

**Carbon doping of cubic GaN by CBr<sub>4</sub>** — ●ELENA TSCHUMAK<sup>1</sup>, HARTWIG PÖTTGEN<sup>1</sup>, OLGA KASDORF<sup>1</sup>, JÖRG SCHÖRMANN<sup>1</sup>, JÜRGEN

W. GERLACH<sup>2</sup>, DONAT J. AS<sup>1</sup>, and KLAUS LISCHKA<sup>1</sup> — <sup>1</sup>Universität Paderborn, Department Physik, Warburger Strasse 100, 33095 Paderborn, Germany — <sup>2</sup>Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstraße 15, 04318 Leipzig

Carbon-doped cubic GaN (c-GaN:C) films were grown by plasma-assisted molecular beam epitaxy using carbon tetrabromide (CBr<sub>4</sub>) as a carbon source. The growth was in situ monitored by reflection high-energy electron diffraction (RHEED). To detect the atomic carbon, the quadrupole mass spectrometer was used. Secondary ion mass spectroscopy (SIMS) was used to quantify the carbon incorporation behavior. The electrical properties of carbon doped c-GaN samples were studied by capacitance-voltage (CV) measurements and Hall-effect measurements between 10-400K. The optical properties of the epilayers were studied by photoluminescence (PL) measurements at room temperature and at 4K.

HL 36.45 Wed 16:30 Poster D

**TEM Investigations on defect terminating SiN interlayers in (Al, In)GaN layer systems on sapphire substrate** — ●MARTIN BEER<sup>1</sup>, JOSEF ZWECK<sup>1</sup>, JOACHIM HERTKORN<sup>2</sup>, FRANK LIPSKI<sup>2</sup>, PETER BRÜCKNER<sup>2</sup>, STEPHAN SCHWAIGER<sup>2</sup>, and FERDINAND SCHOLZ<sup>2</sup> — <sup>1</sup>Universität Ulm, Albert-Einstein-Allee 45, D-89081 Ulm, Germany — <sup>2</sup>Universität Regensburg, Universitätsstr. 31, D-93051 Regensburg, Germany

To decrease the dislocation density in (Al,In)GaN layer systems for LEDs grown on sapphire substrates a defect terminating SiN interlayer was deposited at two different positions in the epitaxial layer grown by MOVPE. In the first series of samples the SiN layer was deposited directly on the AlN Buffer layer, in the second series it was inserted into the GaN layer about 350 nm above the substrate - film interface. The deposition time of the SiN layers was varied between 3 min and 7 min yielding to a fractional coverage of about 60 % to 90 %, respectively. Cross-sectioned samples of the differently grown structures were prepared and afterwards analysed in the TEM, e.g. by means of weak beam dark field imaging and HRTEM. The obtained results will be compared to etch pit density measurements.