HL 36: Poster III

The low temperature phase of succinonitrile — IMAD BELABBAS, JORAN CARLSSON, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 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 towards 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].


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 FESER1, CARSTEN DABIEL2, and VLADIMIR DYAKONOV1,2 — ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Wuerzburg — 1Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Wuerzburg, Am Hubland, D-97074 Wuerzburg

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 organic 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 organic electrolyte as well as on the choice of the conduction salt.

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 electrolytically 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 cm²/Vs.


HL 36.5 Wed 16:30 Poster D Impedance spectroscopy on polymer solar cells — ROLAND ROSCH1, INGO HÖRSELMAANN2, ANDREI HERASIMOVIC3, SUSANNE SCHEINERT2, GERHARD GOHSCH1, and HARALD HOPPM1 — 1Institute of Physics, Ilmenau University of Technology, Weimarer Straße 32, 98693 Ilmenau, Germany — 2Institute of Solid State Electronics, Ilmenau University of Technology, Gustav-Kirchhoff-Str. 1, 98693 Ilmenau, Germany — 3Institute of Science and Technology, 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 barriers, dielectric interlayers, 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-TiO2–nanocrystals and charge transfer in blends with P3HT — ANDREAS SPERLICH1, JAN FRIEDMAN1,2, INGO RIEDEL1,2, CARSTEN DABIEL1, and VLADIMIR DYAKONOV1,2 — 1Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Wuerzburg, Am Hubland, D-97074 Wuerzburg — 2ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Wuerzburg

Light-induced electron spin resonance (L-ESR) studies of photogenerated charge carriers in mesoporous films of TiO2 blended with poly(3-hexylthiophene) (P3HT) were performed. The TiO2-films were produced by sol-gel processes. XRD-measurements confirm anatase-TiO2 as several material 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 Ti3+ and O2− 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$_2$ 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$^1$, BENEDETTA CASU$^2$, ACHIM SCHOLL$^3$, FRIEDRICH REINERT$^4$, and EBEBERHARD UMBACH$^1$ — 1University of Würzburg, Experimental Physics II, Am Hubland, 97074 Würzburg, Germany — 2Inst. 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 reactions with 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$_3$, DIP, CuPc, and PBI-H$_4$. 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 energy difference between the HOMO and LUMO levels in the presence of a hole or electron, respectively, after relaxation has occurred.

HL 36.8 Wed 16:30 Poster D

Characterization of organic photovoltaic cells in comparison with analytic simulations — CHRISTIAN KÖRNER$^{1,2}$, FLORIAN HOLCH$^2$, ACHIM SCHOLL$^3$, CARSTEN DEIBEL$^1$, FRIEDRICH REINERT$^4$, and VLADIMIR DYAKONOV$^1$ — 1Universität Würzburg, Experimentelle Physik VI, 97074 Würzburg — 2Universität 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 Cao 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 SCHAFERHANS, 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 by the classical Mott–Grifﬁth model, which assumes hopping between 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$^1$, THOMAS WEIMANN$^2$, HARTMUT FRIEDRICH$^3$, VADIM G. LYSENKO$^4$, and KARL LEO$^1$ — 1Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany, 2www.iapp.de — 2Physikalisch-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$_2$ / TiO$_2$ DBRs and a $\lambda/2$-layer of the dye system Alq$_3$/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 LOHRMANN$^1$, CARSTEN DEIBEL$^1$, and VLADIMIR DYAKONOV$^{1,2}$ — 1Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg — 2ZAE 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 disordered 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 KRANZ$^1$, MORITZ LITTEK$^{1,2}$, ANDREAS SPERLICH$^1$, CARSTEN DEIBEL$^1$, and VLADIMIR DYAKONOV$^{1,2}$ — 1Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — 2The 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. 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 — BART VANHEURSLAET, GERHARD GOEBBIS, and HARALD HOFFMANN — 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
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.

Effect of polymer solar cell geometry on photovoltaic performance — •BUHRAN MUSIHN1, JOACHIM RENZ2, KARL-HEINZ DREU2, GERHARD GOHSCH3, and HARALD HOPPE1 — 1Institute of Physics, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — 2Electronic 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.

The electronic structure of thin films of the organic molecular semiconductors: zinc phthalocyanine (ZnPc), tin phthalocyanine (SnPc) and lead phthalocyanine (PbPc) has 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 density of states respectively. In particular, resonant soft x-ray emission spectroscopy results in the site-specific C 2p and N 2p partial densities 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 data of density functional calculations will be discussed.

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: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 EMDR. By measuring Rashba frequencies as a function of the spectral position of 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 Rashba frequencies as a function of the resonance field, two frequencies could be clearly separated, which resembles the case of two coupled electron spins.

Refined transmission measurement setup for 2D-terahertz structures and the corresponding structure-property-relationships are discussed in view of solar cell application.

Numerical simulation of organic bulk heterojunction solar cells — •ALEXANDER WAGENFALL1, CARSTEN DIEBEL1, ANDREAS BAUMANN1, and VLADIMIR DYA KovON1,2 — 1Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D–97074 Würzburg — 2The 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, Permeval splitting can be observed. By considering different models for polaron dissociation in the active layer as well as 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.

Effect of vacuum pressure during metal electrode sublimation on polymer solar cell performance — •FLORIAN KÜHNLEINZ, GERHARD GOHSCH, 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 O2 and H2O
photonic crystals — •THOMAS KISSINGER and ANDREI PUMENOV — 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 peculiar 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 reliable 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 — •OLEKSY KIRYIEVO, MORITZ BELETTES, STEFAN WACKEROW, WOLFRAM HERGERT, and HEINRICH GRAENER — Institute of Physics, Martin Luther University Halle-Wittenberg, Von-Seeckendorff-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 by preparing dielectrics to which metallic materials are added. Electric field assisted dissolution method. Laser assisted dissolution or modification of nanoparticle containing areas is an elegant way to form waveguides in the two-dimensional 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. 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 MATYSSEK1, STEFAN MEYER2, WOLFRAM HERGERT1, RÜDIGER WEINER1, and MARTIN ARNOGD2 — 1Institute of Physics, MLU Halle-Wittenberg, Von-Seeckendorff-Platz 1, 06120 Halle — 2Institute 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 nanostuctures are two application areas where methods to calculate electromagnetic fields in complicated structures have to be combined with optimization methods. To this purpose we introduce a genetic FDTD algorithm based on the 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 RALP B. WIERSPOH — 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 phoem were fabricated in such a way 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 emitters. 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 — •STEVEN BURGER, JAN POMPLAIN, FRANK SCHMITT, and LIN ZSCHEBECH — 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 program 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].


HL 36.26 Wed 16:30 Poster D

Quasiperiodic structures in metallic photonic crystals — •CHRISTINA BAUER1, DIETHARD NAU1,2, SERGEI ZHUKOVSKY3, and HARALD GIESSEN1 — 14th Physics Institute, University of Stuttgart, 70550 Stuttgart, Germany — 2Institute of Applied Physics, University of Bonn, 53115 Bonn, Germany — 3Physics 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.


HL 36.27 Wed 16:30 Poster D

Nonlinear Coordinate Transformation as an Extension of the Fourier Modal Method to Finite-Sized Structures — •THOMAS ZEHROWSKI1, SABINE ESSE1,2,3, and KURT BUSCH1,2,3 — 1Institut für Theoretische Festkörperphysik, Universität Karlsruhe (TH), Institut für Theoretische Festkörperforschung (CFN), Universität Karlsruhe — 2Karlsruhe School of 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 STANNIGEL1, MICHAEL KÖNZ1,2,3, JENS NIEGEMANN1,2,3, LASHA TIKHISHVILI1,2,3, and KURT BUSCH1,2,3 — 1Institut für Theoretische Festkörperphysik, Universität Karlsruhe — 2DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — 3Karlsruhe School of Photonics & 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 non-photonics. The results are compared to standard methods such as FDTD.

**Numerical Treatment of Nonlinearities in Higher-Order-Time-Domain Methods** — JAN GIESLER1, JENS NIEGEMANN1,2,3, LASHA KRISHNASHIVILY1,2,3, and KURT BUSCH1,2,3 — 1Institut für Theoretische Festkörperphysik, Universität Karlsruhe — 2DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — 3Karlsruhe 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 high-order discontinuous Galerkin scheme for solving Maxwell’s equations with a Kerr nonlinearity. Our approach is further compared to standard methods such as FDTD.

**Component Analysis and Optimization of Photonic Crystal Based Semiconductor Laser Diodes** — HELMUT ZARSCHUEZ1, LIN ZSCHEIDRICH1,2, JAN POMPLUN1,2, and SVEN BURGER1,2 — 1JCMWave GmbH, Haarer Straße 14a, 85640 Putzbrunn, Germany — 2Zuse 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 crystalline 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).

**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.

**Wannier function based numerical analyses of Photonic-Crystal functional elements incorporating optically anisotropic materials** — PATRICK MACK1,2, DANIEL HERMANN2,3, CHRISTOPH KOLPER2, and KURT BUSCH2,3,4 — 1Institut für Nanotechnologie, Forschungszentrum Karlsruhe — 2Institut für Theoretische Festkörperphysik, Universität Karlsruhe — 3DFG Forschungszentrum Center for Functional Nanostructures (CFN), Universität Karlsruhe — 4Karlsruhe 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.

**Chirp dependent Emission of a fs-pumped Semiconductor Disc Laser** — ECKHARD KÜHN1, ANGELA THRÄHARDT1, STEPHAN W. KOCH1, WOLFGANG STÖLL2, SANGAM CHATTERJEE1, CHRISTOPH LANGE1, WOLFGANG RÜHLE1, WENDEL WOHLHEBEN2, and MARCUS MOTZEK3 — 1Fachbereich Physik, Philipps Universität Marburg, Deutschland — 2Polymer Research, BASF AG Ludwigshafen, Deutschland — 3Fachbereich 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 averaging energy of the detected carriers. By strongly increasing 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 Is exciton-resonance and the position of the quantum well barriers due to excitation induced dephasing. The numerical simulations show good qualitative agreement with the experimental data.

**Dephasing processes in quantum dot microcavity systems** — ANDREA RITTER, CHRISTOPHER GIES, JAN SIEBECK, JAN WIERIG, 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 full 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.

**Highly spatial resolved PL spectroscopy of single dislocations in InGaN/GaN quantum well structures** — JULIA DANKHOF1, MATTHIAS EDER1, CLEMENS VERHEIHL1, ULRICH T. SCHWARZ2, WERNER WEISCHNEIDER1, NIKOLAUS GEMWEISENER3, ANSGAR LAUBSCH2, and BERTHOLD HAHN2 — 1NWF II - Physik, Universität Regensburg, Universitätstraße 31, 93053 Regensburg — 2Ossam 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 107 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 spatial resolved photoluminescence (PL) spectroscopy. We now study the impact of single dislocations on the optical properties of InGaN 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 dependence of temperature and excitation density.

**Influence of Optical Gain on the Spectral and Temporal Characteristics of 405 nm (Al,Ga)N GaN Laser Diodes** — WERNER WEGSCHER, BERTHOLD HAHN, ANGELA THRÄHARDT1, STEPHAN W. KOCH1, WOLFGANG STÖLL2, SANGAM CHATTERJEE1, JAN WIERIG2, FRANK JAHNKE2, and FRANK CICHOS3 — Institut für Theoretische Physik, Universität Bremen

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 107 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 spatial resolved photoluminescence (PL) spectroscopy. We now study the impact of single dislocations on the optical properties of InGaN 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 dependence of temperature and excitation density.
Different Substrates — Bernd Schmidtke1, Tobias Meyer1, Harald Braun1, Ulrich T. Schwarz1, Désirée Queren2, Marc Schilling1, Stephan Lütgert2, and Uwe Strauss2 — NWF II - Physik, Universität Regensburg — Osram Opto Semiconductors GmbH

We investigate the spectral and temporal behaviour of violet (Al,Ga)N 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,Ga)N laser diodes using a rate equation model with nonlinear gain effects. Additionally the gain of each longitudinal modes 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,Ga)N Laser Diodes: Experiment and Simulation — *STEFAN ROGOWSKY1, DOMINIK SCHOLZ1, HARALD BRAUN1, ULRICH T. SCHWARZ1, ANSGAR LAUBRICH2, GEORG BRÜDERL1, and UWE STRAUSS2 — NWF II - Physik, Universität Regensburg — Osram Opto Semiconductors GmbH

In the (Al,Ga)N 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 widths, 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,Ga)N LDs.

HL 36.38 Wed 16:30 Poster D Hall effect measurements on AlInN layers with high Incontent and low Hall mobility — KAY-MICHAEL GÜNTHER, HARTMUT WITTE, CHRISTOPH HUSS, 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 stored charge modulation. Therefore the spatial resolved rate equations for carriers and thermal-induced modifications of the ridge waveguide refractive index profile are solved. The interaction with the optical mode in the modified refractive index profile is included. 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,Ga)N LDs.

HL 36.39 Wed 16:30 Poster D Structural and magnetic properties of Eu-, Ho- and Sm-implanted GaN — FANG-YUN LO1, VERENA NEY2, ANDREAS NEY2, ANDREAS MEITZEN1, OLIVER REIF1, ANDREAS PETERS1, and ANDREAS D. WIECK1,2 — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Bochum, Lehrstät. 150, D-44780 Bochum — 2Experimentalphysik, Universität Duisburg-Essen, Lothrstr. 1, D-47057 Duisburg — RUBION, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum

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, experimental results are quite scattered around 30 K when compared to the theoretical work predicted Curie temperatures. 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 SCHÖRMANN1, ELENA TCHUMAK1, DONAT J. AS1, KLAUS LISCHEK1, ERIC A. DECUR1,2, and OMAR MANASREH2 — 1Department of Physics, University of Paderborn, Warburger Str. 100, 33095 Paderborn — 2Department 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 sample. The magnetic properties of the AlN/GaN 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 μm - 2.0 μm 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 Quantumfilmen mit Photolumineszenz und Röntgenbeugung — TORENST LANGER, HOLGER JÖNEN, LABS HOFFMANN, DANIEL DRANGER, HEIKO BREMMERS, DANIEL FUHRMANN, UWE ROSOW und ANDREAS HANGLEITEN — Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstrasse 2, 38106 Braunschweig

Für optoelektronische Anwendungen im langwelligen Bereich werden InGaN-Quantenfilmen mit hohem Indium-Gehalt von grösser 30% benötigt. Bei so hohem Indium-Gehalt sind jedoch selbst durch relativ kurze Anlagerung durch die exzentrische Lage der GaN (0001)-2 surfaces by oxygen and water — PIERRE LORENZ, RICHARD GUTT, JUERGEN A. SCHRÄFER, and STEFAN KRISCH — Institut für Physik und Institut für Mikro- und Nanotechnologie, 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 2 surfaces by oxygen and water exposure, drastic changes are observed. Upon oxygen exposure, the as-grown samples, two surface states at 2 eV and 3 eV below EF can be found in the ultraviolet photoelectron valence band spectra. For higher exposures, an additional peak at 4 eV appears, which remains constant and the valence band spectrum increases by 0.3 eV and a downward bend bending of 0.4 eV is observed. For higher exposures, a peak at 0.7 eV appears, which remains constant and the valence band spectrum increases by 0.3 eV and a downward bending of 0.4 eV is observed. For higher exposures, a peak at 0.7 eV appears, which remains constant and the valence band spectrum increases by 0.3 eV and a downward bend bending of 0.4 eV is observed. For higher exposures, a peak at 0.7 eV appears, which remains constant and the valence band spectrum increases by 0.3 eV and a downward bend bending of 0.4 eV is observed. For higher exposures, a peak at 0.7 eV appears, which remains constant and the valence band spectrum increases by 0.3 eV and a downward bend bending of 0.4 eV is observed.
shows a comparable behaviour, with a disappearance of the 2 eV surface state after an exposure of 0.2 L.


**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. Fey¹, L. Reißmann¹, F. Schulze¹, A. Dadgar¹,², J. Christen¹ und A. Krost¹,² — ¹Institut für Experimentelle Physik, Otto-von-Guericke-Universität, 39016 Magdeburg — ²AZZURRO Semiconductors AG, Universitätsplatz 2, 39106 Magdeburg


**HL 36.44 Wed 16:30 Poster D**

**Carbon doping of cubic GaN by CBr₄** — ●Elena Tschumak¹, Hartwig Pottgen¹, Olga Kasdorf¹, Jörg Schörmann¹, Jürgen W. Gerlach², Donat J. As¹, and Klaus Lischka³ — ¹Universität Paderborn, Department Physik, Warburger Strasse 100, 33095 Paderborn, Germany — ²Leibniz-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 (CBr₄) as a carbon source. The growth was in situ monitored by reflection high-energy electron diffraction (RHEED). To detect the atomic carbon, the quadrupol 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 Beer¹, Josef Zwick¹, Joachim Hertkorn², Frank Lipski², Peter Brückner², Stephan Schwaiger², and Ferdinand Scholz² — ¹Universität Ulm, Albert-Einstein-Allee 45, D-89081 Ulm, Germany — ²Universität Regensburg, Universitätstr. 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.