HL 57: Optical properties of bulk semiconductors

Time: Wednesday 16:15–18:00 Location: EW 015

HL 57.1 Wed 16:15 EW 015

Quantum defect of the Rydberg series for cuprous oxide — •Florian Schöne, Heinrich Stolz, and Stefan Scheel — Universität Rostock MNF/IfPH, 18055 Rostock, Germany

The bound-state energies of semiconductor excitons are commonly described by the hydrogenic Rydberg formula $E_n = -\mathrm{Ry}/n^2$. However, recent experiments in cuprous oxide[1] have shown that the energy levels for highly excited p-excitons of the yellow series deviate significantly from the established Rydberg formula. Amongst the possible origins of this deviation, such as frequency-dependent background permittivity and coupling to LO-phonons, the largest contributing factor is the nonparabolic shape of the Γ^{7+} valence band. Based on the Suzuki-Hensel-Hamiltonian[2] which covers spin-orbit and magnetic interactions on symmetry grounds, we are able to analytically describe the nonparabolicity of the valence bands. Applying the concept of quantum defects known from atomic physics, the deviations of the resulting bound-state energies from the hydrogenic Rydberg series can be effectively incorporated in a single parameter $\delta_{n,l}$ according to $E_{n,l} = -\mathrm{Ry}/(n-\delta_{n,l})^2$. We will show the results for the calculation of the first Rydberg-Ritz parameters for the lowest angular-momentum exciton states of the yellow series of Cu_2O.

[1] Kazimierczuk, T. *et al.*, Nature **514**, 343-347 (2014)
[2] Suzuki K., Hensel J. C., Phys. Rev. B **9**,4184 (1974)

HL 57.2 Wed 16:30 EW 015

Pulsed magnetic field spectroscopy up to 70 T on the dilute nitride GaAsN — •Faina Esser[1,2], Harald Schneider[1], Stephan Winnerl[1], Oleksiy Drachenko[3], Amalia Patanè[4], Mark Hopkinson[5], and Manfred Helm[1,2] — [1]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]The Laboratoire National des Champs Magnétiques Intenses of Toulouse, France — [4]The University of Nottingham, United Kingdom — [5]The University of Sheffield, United Kingdom

Magnetic fields above 45 T offer great opportunities as a tool for materials research but can only be realized in the pulsed regime. We use pulsed magnetic fields up to 70 T for spectroscopic investigations of the dilute nitride GaAsN. This material is a promising candidate for optical applications because of the possibility for tuning its band gap by the nitrogen content. Our studies focus on the exploration of the band structure and in particular on the determination of the effective mass. Cyclotron-resonance spectroscopy indicates that the effective mass is not strongly affected by nitrogen in comparison to previous publications. Our magneto-photoluminescence investigations reveal the formation of localized and delocalized states as a result of the nitrogen incorporation. Delocalized states undergo transitions to localized ones in very high magnetic fields. This result is in good agreement with a pressure dependent study [1].

[1] J. Endicott, A. Patanè, D. Maude, L. Eaves, M. Hopkinson, and G. Hill, Phys. Rev. B 72, 041306(R) (2005)

HL 57.3 Wed 16:45 EW 015

Giant Magnetic-Field-Induced Third-Harmonic Generation in Semiconductor GaAs — David Brunne[1], •Walter Warkentin[1], Victor Pavlov[2], Roman Pisarev[2], Anna Rodina[2], and Dmitri Yakovlev[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, St. Petersburg, Russia

GaAs has the noncentrosymmetric crystallographic structure of zinc blend type (P.G. $\overline{4}3m$) in which nonlinear optical process of third-harmonic generation (THG) is allowed in the electric dipole approximation. However, an external magnetic field on the order of 10 T gives rise to an enormous enhancement of the THG intensity by a factor of hundred. We observed a resonance in the THG spectra of GaAs in the vicinity of the 1s-excitonic state, which is related to the four-photon THG processes. The observed resonance is attributed to the intricate modification of polariton-excitonic structure in magnetic field mixing dark and bright 1s-excitonic states. Magnetic-field, rotational anisotropy and temperature studies allowed us to unambiguously confirm the magnetic-field-induced THG mechanism in GaAs. It is important that suggested mechanism of the THG enhancement can be valid for other semiconductors as well.

HL 57.4 Wed 17:00 EW 015

Determination of absolute Raman scattering cross sections in wz-GaN — •Christian Röder, Gert Irmer, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany

Reports on relative or absolute Raman scattering cross sections of phonons in wurtzite-type GaN are scarce in literature. Loa *et al.* [1] report on measurements of absolute and relative Raman scattering efficiencies of phonons which are accessible in backscattering geometry. In this work relative Raman scattering efficiencies of all Raman active phonon modes in wz-GaN were obtained using various scattering geometries [2]. Taking the dependence of the scattering cross sections on the phonon frequencies into acount the complete Raman tensors of wz-GaN were ascertained. For the determination of the absolute scattering cross sections comparative measurements with standard substances such as cyclohexane (C_6H_{12}) and carbon tetrachloride (CCl_4) were performed.

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[1] Loa, I. *et al.*: J. Raman Spectrosc. **29**, 291 (1998)
[2] Irmer, G. *et al.*: J. Appl. Phys. accepted

HL 57.5 Wed 17:15 EW 015

First-Principles calculations of the single-particle properties for novel Bismide and Nitride containing III-V semiconductors — •Phil Rosenow[1], Phillip Springer[1], Stephan W. Koch[2], and Ralf Tonner[3] — [1]Research Training Group GRK 1782, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany

Novel, Bi and/or N containing GaAs based semiconductor systems have great potential for optoelectronic applications ranging from lasers, LEDs, solar cells, all the way to detectors.(1) For the systematic microscopic modelling of such devices, it is a prerequisite to have reliable information on the electronic bandstructure and the single-particle wavefunctions of the respective materials. Here, we use DFT with the MBJLDA functional. Using the resulting bandstructure, we used a least-squares fitting procedure to extract $\mathbf{k}\cdot\mathbf{p}$ parameters.(2) Since the extracted $\mathbf{k}\cdot\mathbf{p}$ parameters incorporate the effects of other bands, they are effective parameters allowing to treat systems that have not been experimentally characterized in any way since all parameters can be obtained computationally. Effects of disorder in mixed systems can be treated as well by averaging over various congigurations.

(1) N. Koukourakis *et al.*, *Appl. Phys. Lett.* **2012**, 100, 092107-092103. (2) R. Oszwaldowski, M. Reichelt, T. Meier, S. W. Koch, M. Rohlfing, *Phys. Rev. B* **2005**, 71.

HL 57.6 Wed 17:30 EW 015

Microscopic Calculations of the Optical Properties of Novel Bismide and Nitride Containing III-V Semiconductors — •Phillip Springer[1], Phil Rosenow[1], Ralf Tonner[2], Jörg Hader[3], Jerome Moloney[3], Tineke Stroucken[4], and Stephan W. Koch[4] — [1]Research Training Group GRK 1782, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]NLCSTR Inc., Tucson, Arizona 85705, USA — [4]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany

Using first-principles calculations to determine the single-particle properties of novel dilute Bismide or Nitride systems, we compute the absorption, gain and luminescence properties of such systems. We extract effective $\mathbf{k}\cdot\mathbf{p}$ parameters from DFT calculations which are then utilized to obtain the band structure as well as the optical and Coulomb matrix elements between the relevant valence and conduction bands using a Luttinger anti-crossing model. On this basis, we calculate the optical properties within the framework of the semiconductor Bloch and luminescence equations.

HL 57.7 Wed 17:45 EW 015

Erbium-doped slot waveguides containing Silicon nanocrys-

tals — Romy Hoffmann[1], •Jan Beyer[1], Volker Klemm[2], David Rafaja[2], Brett Johnson[3], Jeffrey C. McCallum[3], and Johannes Heitmann[1] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, D-09596 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, D-09596 Freiberg, Germany — [3]Centre for Quantum Computation and Communication Technology, School of Physics, University of Melbourne, Melbourne, Victoria 3010, Australia

Silicon-based waveguides are intensely investigated with regard to their potential applications in e.g. inter-chip optical data transmission and data manipulation, e.g. as waveguide amplifiers, but also as possible laser sources. A particularly promising device architecture is provided by the slot waveguide geometry, in which a thin SiO_2 slot is inserted into the silicon waveguide. Due to the refractive index contrast, the electric field amplitude polarized normal to the slot plane is enhanced inside the slot, which improves both absorption and emission efficiency of embedded luminescent structures. We incorporate both Erbium ions and size-controlled Silicon nanocrystals, used as Erbium sensitizers, into such a slot. Most efficient pumping of the 1.54 μm Erbium emission is found for small Si nanocrystals, in the range of 3 nm, and elevated post-Er-implantation annealing temperatures of 1000 °C. The sample structure is also demonstrated to induce a dependence on the polarization direction of the exciting laser light, where polarization normal to the slot layer enhances Erbium emission intensity.