HL 79: Poster: New Materials

Time: Thursday 15:00–19:00 Location: P2-OG3

HL 79.1 Thu 15:00 P2-OG3

Exciton recombination dynamics of graphene nanoribbons probed by time-resolved Raman spectroscopy — •Raphael German, Jinghi Zhu, Boris Senkovskiy, Alexander Grüneis, and Paul H.M. van Loosdrecht — II.Physikalisches Institut Köln, Zülpicher Str. 77, 50937 Köln

Graphene based materials show remarkable chemical, electrical and optical properties. Recently, it has been shown that one can grow atomically precise one-dimensional graphene nanoribbons. Here, we investigate armchair graphene nanoribbons of N=7 carbon atoms width transferred onto the insulating substrate, using steady state and time-resolved spontaneous Raman spectroscopy. The Raman signal shows a resonance near 2.2 eV, consistent with the energy level structure. The time-dependent Raman data is interpreted in terms of exciton recombination dynamics, indicating that exciton recombination occurs mainly through exciton-exciton annihilation which is limited by one-dimensional diffusion.

HL 79.2 Thu 15:00 P2-OG3

Comparison of the electrical conductivity between H terminated and heated electronic grade diamonds — •Sven Graus[1], Stefan Borgsdorf[1], Ulrich Köhler[1], Nikolas Wöhrl[2], Dennis Oing[2], Volker Buck[2], Tanmoy Chakraborty[3], and Dieter Suter[3] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr- Universität Bochum, Germany — [2]Experimentalphysik, AG Lorke, Universität Duisburg-Essen, Germany — [3]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially nitrogen vacancy (NV) centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing and are elements for quantum information technologies. We create the NV centers with low energy nitrogen implantation in electronic grade diamonds. To prevent charging effects on the surface which defocus the ion beam it is common to use hydrogen terminated diamonds. The termination in combination with water adsorbates leads to a surface conductivity which is induced by a two dimensional hole gas (2DHG) close to the surface. For implantation experiments at high temperatures (up to 900 °C) the termination and also the 2DHG is destroyed but the conductivity induced by charge carriers from boron impurities and intrinsic charge carries is rising with the temperature. We compared the conductivity by van der Pauw measurements of the terminated diamond at RT and the diamond at 900 °C in UHV. The appearance of any defocusing effects on the hot diamond while implantation were also checked.

HL 79.3 Thu 15:00 P2-OG3

UHV nanopositioning system for close to surface nitrogen implantation in diamond — •Stefan Borgsdorf[1], Ulrich Köhler[1], Tanmoy Chakraborty[2], and Dieter Suter[2] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr- Universität Bochum, Germany — [2]Experimentelle Physik IIIA, Technische Universität Dortmund, Germany

Color centers in diamond, especially nitrogen vacancy (NV) centers, are practical single photon emitters due to RT operation and are candidates for applications in quantum computing and are elements for quantum information technologies. We present a setup for low energy implantation of NV centers near to the surface with a lateral resolution from micrometer to nanometer scale. The lateral resolution is achieved by a closed loop nanopositioning system combined with an exchangeable aperture with diameters between a micrometer down to a few nanometer. The system allows us to heat the sample up to 900 °C in UHV while implanting with nitrogen without any graphitization on the surface.

HL 79.4 Thu 15:00 P2-OG3

Macro- and micro-scale investigation of diamond etching — •Meng Ge, Christian Osterkamp, Fedor Jelezko, and Alexander Kubanek — Institute for Quantum Optics, Ulm University, D-89081 Ulm, Germany

Diamonds have special usage in quantum information science and technology. The existence of the negatively charged nitrogen-vacancy (NV) centers in diamond, whose electron spin can be coherently manipulated by microwave, are very good candidates for single photon sources, nano-scale magnetic and electric field sensors, and quantum bits (qubits). For many applications good optical and spin properties are required in micro-and nanostructured diamond devices. In order to fulfill this aim and provide a smooth and uniform method, plasma processes are employed. During our research, we focus on both the SF6 and the O2 inductively coupled plasma (ICP) processes.We optimize etching process towards fabrication of diamond nano-structures. A confocal microscope is used for characterizing NV centers in our diamond before and after the diamond structuring procedure.

HL 79.5 Thu 15:00 P2-OG3

Robust optically pumped nuclear spin polarization — •Jochen Scheuer[1], Ilai Schwartz[2], Samuel Müller[1], Qiong Chen[2], Martin B Plenio[2], Boris Naydenov[1], and Fedor Jelezko[1] — [1]Institute of Quantum Optics, Ulm University, Ulm, Germany — [2]Institute of Theoretical Physics, Ulm University, Ulm, Germany

Dynamical nuclear polarisation (DNP) can enhance the sensitivity of magnetic nuclear resonance imaging (MRI) by several orders of magnitude. Nanodiamonds are candidates for novel MRI tracers with particle sensitivity and long coherence times. There are several techniques which perform well for hyperpolarization in aligned magnetic fields, however, they are not applicable for randomly oriented nanodiamonds at ambient conditions. Here polarization and read out of a ^{13}C nuclear spin bath is demonstrated by using a single nitrogen-vacancy (NV) center in a macroscopic diamond.

Our polarization methods use microwave dressed states and semi-adiabatic passages to transfer the NV's electron spin polarization to the surrounding carbon nuclear spins, whereas the NV is repeatedly polarized optically.

We show that using integrated solid effect both for single and double quantum transitions a nuclear spin polarization can be achieved for broadened NV-ESR lines e.g. when the static magnetic field is not aligned along the NV's crystal axis [1]. Our results can be applied for DNP in nanodiamonds, which would find a wide application in magnetic resonance imaging and could revolutionize the field.

[1] Chen, Q., et al., Phys Rev B 92.18 (2015): 184420.

HL 79.6 Thu 15:00 P2-OG3

Sensing Properties of Carbon-Nanotube/Boron-Nitride-Nanotube Heterojunction towards Carbon Monoxide: A First Principles Study — •Shahim Vedaei and Ebrahim Nadimi — Center for Computational Micro and Nanoelectronics, Faculty of Electrical Engineering, K. N. Toosi University of Technology, Tehran, Iran

Detection of carbon monoxide (CO), known as silent killer, is of great importance. Nanotubes could be considered as useful materials for gas sensing applications due to their large surface to volume ratio. But carbon nanotubes (CNT) have almost no interaction with CO molecule and boron nitride nanotubes (BNNT) shows small binding energy of about 0.2 eV. However, we find that, the CNT/BNNT/CNT heterojunctions with appropriate BNNT length show binding energies with CO of the order of 1 eV. The calculations have been performed within pseudopotential density functional theory (DFT) as implemented in SIESTA code. Non-stoichiometric BNNT layers as well as interface bonding (N-C or B-C) could strongly influence the adsorption energy and consequently the sensing behavior. The results show that such heterojunction could be a promising candidate for CO detection.

HL 79.7 Thu 15:00 P2-OG3

Nanostructured water and carbon dioxide inside collapsing carbon nanotubes at high pressure — •Wenwewn Cui[1], Tiago Cerqueira[2,1], Silvana Botti[2,3], and Miguel Marques[4,3] — [1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]European Theoretical Spectroscopy Facility — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

We present simulations of the collapse under hydrostatic pressure of carbon nanotubes containing either water or carbon dioxide. We show that the molecules inside the tube alter the dynamics of the collapse

process, providing either mechanical support and increasing the collapse pressure, or reducing mechanical stability. At the same time the nanotube acts as a nanoanvil, and the confinement leads to the nanostructuring of the molecules inside the collapsed tube. In this way, depending on the pressure and on the concentration of water or carbon dioxide inside the nanotube, we observe the formation of 1D molecular chains, 2D nanoribbons, and even molecular single and multi-wall nanotubes. The structure of the encapsulated molecules correlates with the mechanical response of the nanotube, opening opportunities for the development of new devices or composite materials. Our analysis is quite general and it can be extended to other molecules in carbon nanotube nanoanvils, providing a strategy to obtain a variety of nanoobjects with controlled features

HL 79.8 Thu 15:00 P2-OG3

EPR spectroscopy of Yb3+ in lithium yttrium borate (LYB) single crystals — •Sara Arceiz Casas[1], Gábor Corradi[2], László Kovács[2], Éva Tichy-Rács[2], and Sigmund Greulich-Weber[1] — [1]Paderborn University, Warburger Str. 100, 33098 Paderborn, Germany — [2]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Konkoly-Thege u. 29-33, 1121 Budapest, Hungary

Lithium yttrium borate Li6Y(BO3)3 is an excellent nonlinear optical material with a wide UV range of transparency. Due to the easy incorporation of rare earth ions at Y sites LYB is a prospective laser host material. Yb3+ ions are especially interesting for near-infrared laser pulse applications, indeed, mode-locked and Q-switched laser operation near 1042 nm in Yb-doped LYB has already been realized. EPR studies of Yb+3 in LYB have only been reported in powdered materials. Here single-crystal results on the EPR and its temperature dependence characterizing the Stark-split ground state of Yb+3 in the low symmetry crystal field of LYB are presented.

LYB crystals doped with 1 mol% Yb were grown by the Czochralski method. EPR was measured at low temperature on samples oriented by X-ray diffraction and cut perpendicular to the crystallographic twofold symmetry axis b. Angular dependent EPR spectra near 5K have been taken for the magnetic field in four crystallographic planes required for a full and unambiguous determination of the g-tensor and the hyperfine-tensor of the 171Yb and 173Yb isotopes. The results show reasonable agreement with theoretical results published recently.

HL 79.9 Thu 15:00 P2-OG3

Theoretical and experimental investigation of Iron doped hexagonal $BaTiO_3$ — •Waheed A. Adeagbo[1], Sanjeev K. Nayak[2], Hichem B. Hamed[1], Hans T. Langhammer[3], Wolfram Hergert[1], and Thomas Müller[4] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [2]Department of Materials Science and Engineering, University of Connecticut, USA — [3]Institute of Chemistry, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany — [4]Faculty of Physics and Earth Sciences, Leipzig University, 04103 Leipzig, Germany

EPR measurements on Fe-doped hexgonal $BaTiO_3$ (h-BTO), with Fe concentration between 0.5−2.0 mol%, show the detection of isolated Fe^{3+} which occupies only one of the two crystallographic different Ti sites, that could be the exclusively corner-sharing octahedron, in all different annealing prepared samples. Also, there is speculation about EPR non-detectable states of Fe^{2+} and Fe^{4+} presence, but Fe^{5+} formation is completely ruled out. Recent further defect center detected is identified as Fe^{3+} associated with an oxygen vacancy (V_O) in the first coordination sphere. The exact Fe^{3+} and V_O occupation sites and the V_O roles in the complex are still unknown. Thus, we have used the first principles approach to study the defect properties of substitutionally doped Fe in h-BTO and to examine the role played by the V_O in structure, electronic and magnetic properties due to the introduced defects in the pure crystal. Our theoretical analysis of the defect formation energy derived from the total energies of defective supercells in various charge states will be presented with respect to available EPR-data.

HL 79.10 Thu 15:00 P2-OG3

structural engineering of electrode materials for Na-ion batteries — •Benrong Hai[1,2], Yang Xu[1], Min Zhou[1], Chengliang Wang[1], Liying Liang[1], Yan Mi[1], and Yong Lei[1] — [1]TU-ilmenau, Ilmenau, Germany — [2]Northeastern University, Shenyang, P. R. China

In response to the increased demands of energy storage, Na-ion batteries (SIBs) appear as alternatives to lithium ion batteries. However, because of large radius of Na ions, more complex requirements for the intrinsic properties raise the difficulties in finding a suitable material. Structural engineering is a promising approach to enhance sodium storage, of which amorphization and introduction of oxygen vacancies are two efficient methods to allow the crystalline features of active materials more suitable for large sodium ions. For the former method, TiO2 electrodes with different orderliness of atomic arrangement are employed as the state-of-the art example. Corresponding results prove that the disordering at the surface is benefit for the faradaic contribution from surface processes, which is particularly significant to the electrode materials with poorer affinity of transporting ions. With regard to the influences of oxygen vacancies (OVs), the SIB performance of MoO3 and amorphous SnO2 with and without OVs both evidence that the OVs can increase the electric conductivity and Na-ion diffusion coefficient, leading to the promotion of sodium storage.

HL 79.11 Thu 15:00 P2-OG3

A New Concept for Doping Silicon and its Nanostructures: Modulation Doping using Al-induced Acceptor States in SiO2 — •Daniel Hiller[1] and Dirk König[2] — [1]Laboratory for Nanotechnology, IMTEK, University of Freiburg, Germany — [2]University of New South Wales (UNSW), Sydney, Australia

Silicon nanostructures are omnipresent in fundamental research (quantum dots, nanowires) but are also approached in future technology nodes of the microelectronics industry. Several fundamental physical principles based on diffusion, statistics, and quantum confinement, impede efficient and reproducible impurity doping of nano-Si with e.g. P or B.

In this presentation, we highlight a novel concept: Heterostructure modulation doping of Si using an acceptor state of Al-atoms in SiO2. This state is located 0.5 eV below the Si valence band and captures electrons from the Si over a distance of several nanometers, leaving behind holes as majority carriers [1]. We demonstrate experimental evidences of this mechanism: fixed negative charges and increased tunnelling currents in SiO2:Al thin films, induced holes in modulation doped Si quantum wells, and PL quenching of modulation doped Si nanocrystals.

[1] D. König & D. Hiller et al., Sci. Rep., under review (2016)

HL 79.12 Thu 15:00 P2-OG3

Designing Locally Symmetric Eigenstates in Planar Discrete Systems — •Malte Röntgen, Christian V. Morfonios, and Peter Schmelcher — Zentrum f. Optische Quantentechnologien, Luruper Chaussee 149, 22761 Hamburg

Local symmetries are spatial symmetries that are only present in a spatially finite subdomain of a system. Contrary to the usual case of global symmetries, the effects of local symmetries on the system's eigenstates are not obvious and thus have not been investigated thoroughly in the past. However, in this paper we show that it is indeed possible to gain knowledge about the structure of the eigenstates of systems possessing local symmetries. To this end, we use and extend a framework of so-called non-local currents that has been established recently. The then-extended framework is applicable to all kinds of discrete planar Schrödinger systems, including those with non-uniform connectivity. We use the framework both to derive general identities as well as to investigate two locally symmetric subsystems in detail. These subsystems are closed-loops and one-dimensional open ended chains. We find that, depending on the local symmetry and the type of subsystem, some or all amplitudes within the subsystem to be related by a constant factor. Since these effects can easily be understood using our framework of non-local currents, we expect it to help researchers finding and understanding more effects of local symmetries.

HL 79.13 Thu 15:00 P2-OG3

Optical properties of (CuI)-based inorganic-organic hybrid materials as active semiconductor in planar microcavities — •Lukas Trefflich[1], Gabriele Benndorf[1], Rüdiger Schmidt-Grund[1], Harald Krautscheid[2], and Marius Grundmann[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Institute for Inorganic Chemistry, University of Leipzig, 04103 Leipzig, Germany

We have investigated electronic and optical properties as well as temporal dynamics of (CuI)-based inorganic-organic hybrid materials using photoluminescence spectroscopy and ellipsometry. By changing the chemical composition bright light emission in the visible spectral range can be tuned from approximately 450 nm to 650 nm . We found the luminescence decay time to be in the microsecond range. Furthermore, we have determined the dielectric function from the far UV to

mid IR range in order to design planar microcavities for possible laser and LED application. This is of particular interest because white light LEDs usually contain rare-earth elements. [1] Their mining is difficult and expensive. Because of the facile synthesis, high quantum yield (up to 95%), thermal stability and optical tunability [2], (CuI)-based inorganic-organic hybrid materials are promising alternatives.
[1] H. Höppe, Angew. Chem., Int. Ed. 2009, 48, 3572
[2] W. Liu et al., J. Am. Chem. Soc. 2015, 137, 9400-9408

HL 79.14 Thu 15:00 P2-OG3

Structural and optical properties of TiN/MgO superlattices — •Florian Jung, Vitaly Zviagin, Michael Bonholzer, Chris Sturm, Jörg Lenzner, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

We present an investigation of structural and optical properties of TiN/MgO superlattices grown by pulsed laser deposition on MgO(100)-substrates. Multilayers and superlattices are grown in an argon atmosphere and their growth is in-situ monitored using reflection high energy electron diffraction. The films' structural properties are evaluated using X-ray diffraction, X-ray reflectometry, atomic force microscopy and reciprocal space mapping techniques. Systematic studies of the dependence of optical properties of the films on process parameters are performed using ellipsometry.

Periodic metal/dielectric planar metamaterials are known to be adjustable such that they exhibit a hyperbolic dispersion and thus anisotropic optical behaviour. Material stacks on a sub-wavelength scale realising such a dispersion are referred to as hyperbolic metamaterials (HMMs). Titanium nitride has already been applied as a plasmonic component in previous studies[1]. Our results show, that MgO/TiN superlattices are promising for application as HMMs.

[1] G. V. Naik et al., PNAS, Vol. 111, No. 21, 7546-7551 (2014)

HL 79.15 Thu 15:00 P2-OG3

Band Offset in (Ga,In)As/GaAs/Ga(As,Sb) heterostructures — Sebastian Gies[1], •Benjamin Holz[1], Maria Weseloh[1], Christian Fuchs[1], Wolfgang Stolz[1], Jörg Hader[2,3], Jerome Moloney[2,3], Stephan Koch[1], and Wolfram Heimbrodt[1] — [1]Department of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Nonlinear Control Strategies Inc., 7040 Montecatina Dr., Tucson, AZ 85704, USA — [3]College of Optical Sciences, University of Arizona, Tucson, AZ 85721, USA

The (Ga,In)As/GaAs/Ga(As,Sb) material system is used for lasers operating over a wide spectral range in the infrared. To further optimize the design of such heterostructures, it is important to have exact knowledge of the band structure and the band offsets, in particular. Here, we present a thorough analysis of the optical properties of (Ga,In)As/Ga(As,Sb) type-II heterostructures by means of temperature- and power-dependent photoluminescence spectroscopy. In conjunction with a microscopic many-body theory we are able to determine the band offset between Ga(As,Sb) and GaAs with high precision. Furthermore, we reveal the temperature dependent band-alignment in these heterostructures. Additionally, we introduce a GaAs interlayer of variable thickness to influence the tunnel processes of the charge carriers. Here, the great importance of these tunneling processes on the optical spectra and the influence of the internal interfaces are investigated.

HL 79.16 Thu 15:00 P2-OG3

Calculation of forces in the KKR method — •Jonas Friedrich Schäfer, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität Gießen

Although the general method of calculating forces on atomic nuclei in the KKR formalism seems to be simple, a closer investigation reveals major challenges: First, Hellmann-Feynman forces are very sensitive to small deviations from a spherical core electron density. Given that spherical symmetry is a requirement for fast convergence of the angular momentum expansion, this contribution needs special treatment. Further, the expression for the interstitial space contribution (i.e., the space outside the Muffin-Tin spheres) is highly sensitive to the angular momentum cut-off, too. We present quantitative studies to the aforementioned problems and trace them back to the underlying mathematical expressions. Based thereupon, we discuss possible improvements to the calculational scheme.

HL 79.17 Thu 15:00 P2-OG3

Elastic strain relaxation and evolution in GaAs/InGaAs/GaAs radial nanowire heterostructures — •Ali Al Hassan[1], Ryan B. Lewis[2], Hanno Küpers[2], Emmanouil Dimakis[2], Arman Davtyan[1], Christian Sternemann[3], Abbes Tahraoui[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Naturwissenschaftlich-Technische Fakultät der Universität Siegen, 57068 Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [3]Zentrum fuer Synchrotronstrahlung Technische Universitaet Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

The optical performance of nanowire based devices is strongly related to the sharpness of the hetero-interface and the homogeneity of atomic composition within the active volume. In GaAs/InGaAs/GaAs core-shell-shell nanowires, misfit strain can easily release towards NW side planes. However due to hexagonal geometry of the nanowires, the interfacial strain might differ towards different radial directions and requires careful analysis. Towards this goal, we report explicitly on the 3D investigation of the strain interaction and relaxation mechanisms in GaAs/InGaAs/GaAs core-shell-shell NW ensembles by means of high resolution x-ray diffraction (XRD) and finite element methods (FEM) as a function of InGaAs shell thickness and nominal indium concentration. In order to obtain a full 3D strain field map, special attention was paid to determine the strain impact along the azimuth and in-plane directions of the NW core shell system.

HL 79.18 Thu 15:00 P2-OG3

Transmission Electron Microscopy investigations on structural origins of cross hatching in $Si_{1-x}Ge_x$/Si — Florian Biebl, •Elisabeth Anna Zolnowski, Felix Schwarzhuber, Christian Neumann, Michaela Trottmann, Dominique Bougeard, and Josef Zweck — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The occurrence of cross-hatched surfaces can be observed under certain growth conditions in various strain engineered semiconductor materials. This means, that a surface shows periodic ridges and trenches along specific growth directions. This phenomenon influences the electron mobility and other properties of the grown materials. Therefore, it is important to understand the origin of the cross-hatch pattern (CHP) in order to prevent unwanted effects in semiconductor devices. By Transmission Electron Microscopy (TEM) we investigated CHPs on epitaxially grown strain-relaxed $Si_{1-x}Ge_x$/Si by molecular beam epitaxy, prepared as a cross section specimen along a periodic direction of the CHP. The periodicity and depth of the CHP observed in our measurements are in good agreement with literature [1]. Further, we could show that there is a correlation between the occurrence of a trench and a so called 60° dislocation originating in the substrate. In addition, we will present results of nanodiffraction experiments, revealing that these dislocations may separate areas of slightly different crystallographic orientations.
[1] Lutz et al., Influence of misfit dislocations on the surface morphology of $Si_{1-x}Ge_x$ films, Applied Physics Letters 66, 724 (1995)

HL 79.19 Thu 15:00 P2-OG3

Effect of the different surface texture on the metal-insulator-silicon photoanodes performances for water photosplitting — •Haojie Zhang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

Metallurgical grade (MG) silicon processed with the metal-assisted chemical etching(MaCE) can not only promote the purity, but also from the nanostructures in the bulk of the MG silicon. Since the surface texture of the silicon was dominated the optical (e.g. reflection, scattering, carries, bending gap and charge-transfer rate) and chemical (e.g. catalytic site, surface area and defects) characteristics. Moreover, the stability in extremely acidic and basic electrolytes was concerned and could be effectively enhanced by coating a thin and robust tunneling layer (such TiO2, ZnO). Herein, the different texture surfaces of Si were demonstrated by MaCE with different catalytic and other methods as a comparison. A protecting layer and catalytic particles were deposited by Atomic Layer Deposition (ALD) to promote the durable and catalytic performance in the photoelectrochemical(PEC).

HL 79.20 Thu 15:00 P2-OG3

Comparison of Cu, Ag and Pt assisted chemical etching for metallurgical silicon purification — •Junna Wang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2]

— [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

The purity of metallurgical grade silicon can be improved during metal assisted chemical etching (MaCE). Since MaCE can form nanostructures in metallurgical silicon (MG Si), metal impurities are removed during the formation of porous silicon. We chose different catalytic metals and compared the resulting nanostructures moreover the catalyst selection results in different purification efficiency and application.

HL 79.21 Thu 15:00 P2-OG3

Effect of the different surface texture on the metal-insulator-silicon photoanodes performances for water photosplitting. — •Haojie Zhang[1,2], Stefan L. Schweizer[1], Alexander Sprafke[1], and Ralf B. Wehrspohn[1,2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Fraunhofer-Institut für Mikrostruktur von Werkstoffen und Systemen IMWS

Metallurgical grade (MG) silicon processed with the metal-assisted chemical etching(MaCE) can not only promote the purity, but also from the nanostructures in the bulk of the MG silicon. Since the surface texture of the silicon was dominated the optical (e.g. reflection, scattering, carries, bending gap and charge-transfer rate) and chemical (e.g. catalytic site, surface area and defects) characteristics. Moreover, the stability in extremely acidic and basic electrolytes was concerned and could be effectively enhanced by coating a thin and robust tunneling layer (such TiO2, ZnO). Herein, the different texture surfaces of Si were demonstrated by MaCE with different catalytic and other methods as a comparison. A protecting layer and catalytic particles were deposited by Atomic Layer Deposition (ALD) to promote the durable and catalytic performance in the photoelectrochemical(PEC).

HL 79.22 Thu 15:00 P2-OG3

Anneal induced transforms of radiation defects in heavily irradiated Si detectors — •Dovile Meskauskaite, Tomas Ceponis, Eugenijus Gaubas, Vytautas Rumbauskas, and Juozas Vaitkus — Vilnius University Institute of Applied Research, Vilnius, Lithuania

In this research, transforms of the radiation defect induced by anneals have been studied in heavily irradiated Si. The n-type and p-type CZ and FZ Si material samples and detector structures, irradiated by high energy electrons (6.6 MeV), protons (26 GeV/c) and pions (300 MeV/c) using fluences up to 5×10^{16} cm^{-2}, have been studied. The deep level spectra have been examined by combining the capacitance and current deep level transient spectroscopy (DLTS) and using the optical injection techniques. The DLTS spectroscopy means has been combined with measurements of the temperature dependent carrier trapping lifetime (TDTL). The latter TDTL technique is a contact-less spectroscopy tool based on recording of the microwave-probed photoconductivity transients. This TDTL technique is preferential when radiation trap density approaches or exceeds the dopant concentration and when necessary to avoid modification of a detector structure due to anneals at elevated temperatures. A good agreement between the DLTS and TDTL spectra has been obtained. The dominant radiation defects and their transform paths under isochronal anneals have been revealed.

HL 79.23 Thu 15:00 P2-OG3

Micro-Raman spectroscopy of laser-annealed reheated SiO_x films on silica substrate — •Christian Gobert[1], Nan Wang[1], Thomas Fricke-Begemann[2], Jürgen Ihlemann[2], and Michael Seibt[1] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]Laser-Laboratorium Göttingen, Germany

The development of Si-based opto-electronics for integrated circuits is still an unsolved problem as bulk-Si is an indirect semiconductor resulting in improbable optical transitions. Nanocrystalline silicon (nc-Si) is expected to be a feasible material for this purpose due to quantum confinement effects compassing the indirect band gap [1]. It was recently shown [2] that cw laser irradiation of substrate-bound silicon-rich silicon oxide (SRSO) is suitable to produce a phase separation reaction leading to strong room temperature photoluminescence (PL). The latter was attributed to small amorphous Si clusters in the remaining amorphous silicon oxide matrix, as indicated by Raman spectroscopy. Such particles, however, could not be confirmed by transmission electron microscopy.

In this work, the effect of subsequent low-temperature furnace annealing of laser-annealed SiO_x films on silica substrate is investigated by micro-Raman spectroscopy. In order to test the above hypothesis, changes in Raman spectra induced by low temperature (500-700°C) furnace annealing are followed to observe the selective crystallization of a-Si clusters. [1] T. Nikitin, L. Khriachtchev, Nanomaterials 5, 614-655 (2015) [2] T. Fricke-Begemann, N. Wang, P. Peretzki, M. Seibt, J. Ihlemann, J. Appl. Phys. 118, 124308 (2015)

HL 79.24 Thu 15:00 P2-OG3

Crystal structure and thermoelectric properties of some indium-based thiospinels — •Pawel Wyzga[1,2], Igor Veremchuk[2], Matej Bobnar[2], Tina Weigel[1], Tilmann Leisegang[1], Andreas Leithe-Jasper[2], and Roman Gumeniuk[1] — [1]TU Bergakademie Freiberg, Germany — [2]MPI Chemische Physik fester Stoffe, Dresden, Germany

Nowadays, a particular emphasis in thermoelectric research is put on the obtaining both high-performance and earth abundant materials. These requirements are perfectly suited in case of sulphur-containing materials. For instance, the nonstoichiometric chalcocite $Cu_{2-x}S$ ($x = 0.03$) reveals extremely high values of thermoelectric figure of merit $ZT_{max} = 1.9$ at 970 K [1]. The indium-containing thiospinels MIn_2S_4 (M = Cr, Mn, Fe, Co) [2], initially attracted a special attention due to their interesting magnetic behaviours. In this work, we focus on the study of thermoelectric properties of new $Ti_{0.8}In_{2.2}S_4$ and known $Fe_{0.9}In_{2.1}S_4$ compounds. Both of them show different transport properties: Ti-containing is a metal while that with Fe is a semiconductor. Despite relatively low thermal conductivities at elevated temperatures, both thiospinels show negligibly small ZT values (5×10^{-3} and 2×10^{-3} at 300 K, respectively). However, taking into account that the transport properties of Ti-Fe indium-thiospinels are ranging from metallic to semiconducting, a possibility of tuning of thermoelectric properties makes these sulphides promising materials.

[1] L. Zhao et al., J. Mater. Chem. A 3 (2015) 9432-9437
[2] H. Hahn, W. Klinger, Z. Anorg. Allg. Chem. 263 (1950) 177-190

HL 79.25 Thu 15:00 P2-OG3

Temperature-dependent Seebeck coefficient of silver nanowires — •Maximilian Kockert[1], Danny Kojda[1], Rüdiger Mitdank[1], Johannes Ruhhammer[2], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], Toni Markurt[3], and Saskia F. Fischer[1] — [1]Group Novel Materials, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg — [3]Leibniz-Institute for Crystal Growth, D-12489 Berlin

Bulk silver has the highest electrical and thermal conductivity of all metals. The process of miniaturization and nanopatterning affects these two parameters. The electrical and thermal conductivity of individual silver nanowires were recently investigated in [1] and [2].

In this work, we present the temperature-dependent Seebeck coefficient of individual silver nanowires relative to platinum between temperatures of 10 K and 300 K. The silver nanowires were prepared by the reduction of high purity silver nitrate (99.9999 %). Four individual silver nanowires showed reproducable results. Above 160 K, the diffusive part of the Seebeck coefficent of silver nanowires relative to nanostructured platinum conducting lines $S^{NW}_{Ag,Pt}$ is in agreement with the Seebeck coefficent of bulk silver relative to bulk platinum $S^{Bulk}_{Ag,Pt}$. A change of sign of the Seebeck coefficent takes place at 160 K. Below 160 K, the Seebeck coefficent is dominated by the phonon drag effect.In this regime $S^{NW}_{Ag,Pt}$ differs from $S^{Bulk}_{Ag,Pt}$.

[1] D. Kojda *et al.*, Physical Review B **91**, 024302-1 (2015).
[2] D. Kojda *et al.*, Physica Status Solidi A **213**, 557 (2015).

HL 79.26 Thu 15:00 P2-OG3

Role of interlayer coupling for the power factor of $CuSbS_2$ and $CuSbSe_2$ — •Najebah Alsaleh, Nirpendra Singh, and Udo Schwingenschlogl — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

The electronic and transport properties of bulk and monolayer $CuSbS_2$ and $CuSbSe_2$ are determined by using density functional theory and semiclassical Boltzmann transport theory, in order to investigate the role of the interlayer coupling for the thermoelectric properties. The calculated band gaps of the bulk compounds are in agreement with experiments and significantly higher than those of the monolayers, which thus show lower Seebeck coefficients. Since also the electrical conductivity is lower, the monolayers are characterised by lower power factors. Therefore, interlayer coupling is found to be essential for the excellent

thermoelectric response of $CuSbS_2$ and $CuSbSe_2$ even though it is weak.

HL 79.27 Thu 15:00 P2-OG3

Electronic properties of the thermoelectric Mg2X (X=Si,Ge,Sn)-based alloys — •Juan Guerra, Carsten Mahr, Marcel Giar, Michael Czerner, and Christian Heiliger — Justus Liebig University Giessen, Institut für Theoretische Physik, Giessen, Germany

Since there has been recent research interest in Mg2X based alloy systems for thermoelectric applications, we present an ab initio description of electronic properties in the cases of X=Si, Ge, and Sn. Due to a reported importance of spin-orbit coupling we model the system using a fully relativistic implementation of the density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function method in conjunction with the coherent potential approximation (CPA), which allows us to efficiently account for scattering processes in substitutional alloys. Using our calculation scheme we extract parameters important for transport modelling, e.g. band gaps, charge carrier effective masses and velocities

HL 79.28 Thu 15:00 P2-OG3

Magnetotransport experiments on Lorentz systems with varying scatterer shape — •Tabea Heckenthaler — Heinrich-Heine-Universität Düsseldorf

In the Lorentz model one usually assumes an array of randomly distributed hard disks to model scattering in solids. This has hitherto been discussed primarily from a theoretical point of view.

Due to advancements in semiconductor processing, one can nowadays realize systems with desired specifications in order to also study them experimentally.

We examine such samples based on high electron mobility Ga[Al]As heterostructures, where holes of varying shape are introduced via Ar - ion etching. The scattering at the artificial obstacles dominates the magnetoresistance at low magnetic fields, since background scattering is minimized. We show that these effects have a classical character, which is plausible due to the scatterer size in comparison to the Fermi wavelength.

In addition to the shape we vary the size and density of scatterers and study the effect on magnetoresistance at low temperatures.

HL 79.29 Thu 15:00 P2-OG3

Electron flow focusing with magnetic barriers in 2DEG — •Jan Steimann, Mihai Cerchez, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf

Electrons in a 2DEG are forced to travel from source to drain through two parallel openings in a transversal potential wall, produced by local anodic oxidation. A magnetic barrier is positioned at the openings to control the electron flow. The magnetic barrier height can be tuned such that a number of electrons coming through one opening can be focused onto the second opening, leading to magnetoresistance fluctuations. Experimental results and simulations will be presented.

HL 79.30 Thu 15:00 P2-OG3

Electrical Measurements of Single As-Grown Semiconductor Core-Shell Nanowires — •Danial Bahrami[1], Jovana Colvin[2], Hanno Küpers[3], Rainer Timm[2], Lutz Geelhaar[3], and Ullrich Pietsch[1] — [1]University of Siegen, Solid State Physics department , Siegen, Germany — [2]Lund University, NanoLund and division of Synchrotron Radiation Research, Lund, Sweden — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Characterizing and controlling the electrical properties of core-shell nanowire (NW) heterostructures is fundamental for their implementation into device applications including photonics, sensors, and electronics. For typical conductivity studies, the NW, after removal from the original substrate, is deposited horizontally and contacted with electrodes in as-called field-effect transistor geometry. Here, we report on electrical measurements at single NWs in their as-grown geometry on the substrate by means of FIB/SEM and AFM systems. Using either a tungsten nano-manipulator probe installed inside the FIB/SEM chamber or a sharp metallic tip of a conductive AFM, the I-V curves and current maps along the side-wall and on the top of selected GaAs/InGaAs core-shell NWs have been measured. Similar to previous studies [1, 2], significant differences between the I-V characteristics from individual NWs grown on the same substrate are observed, confirming the necessity of thorough characterization at the single-NW level. The electrical characteristics of NWs can be correlated to their structural properties.

[1] R.Timm et al. Nano Lett. 2013, 13, 5182 -5189. [2] G.Bussone et al. Nano Lett. 2015, 15, 981-989.

HL 79.31 Thu 15:00 P2-OG3

Experimental study of Memory effects in Lorentz Gases — •Matthias Hund[1], Jakob Schluck[1], Thomas Heinzel[1], Klaus Pierz[2], and Hans W. Schumacher[2] — [1]Heinrich-Heine Universität — [2]PTB Braunschweig

The classical Lorentz model is a fundamental class of systems to study transport properties in disordered media. It consists of non-interacting point particles that move through randomly placed static scatterers with short range forces. For such systems, extensive predictions exist for the low density regime, while studies related to large scatterer densities are rare. Resistivity contributions due to scattering correlations are called memory effects. They are expected to modify in particular the magnetoresistivity. Here, we report magnetotransport measurements of Lorentz gases defined with various scatterer densities in high electron mobility $GaAs/Ga_xAl_{1-x}As$ and show that the systems have a characteristic magnetoresistivity which can be attributed to different types of memory contributions.