# HL 84: Poster: Electronic structure theory / Carbon (other than graphene) / Si, Ge, and SiC / III-V semiconductors (other than nitrides)

Time: Wednesday 17:00-20:00

HL 84.1 Wed 17:00 P1

Analytic evaluation of the electronic self-energy in the GW approximation for two electrons on a sphere — •ARNO SCHINDL-MAYR — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The GW approximation for the electronic self-energy is a very important tool for the quantitative prediction of excited states in solids. However, its mathematical exploration has been hampered by the fact that it must, in general, be evaluated numerically even for very simple systems. Here I describe a nontrivial continuum model, consisting of two interacting electrons on the surface of a sphere, and show that a completely analytic derivation of the GW self-energy, in the absence of self-consistency, is possible in this case. In contrast to lattice Hubbard models with the same property, the electron dynamics are governed by the normal long-range Coulomb potential instead of a short-range onsite interaction, the strength of the correlation can be controlled by a natural physical parameter, the sphere radius, and the infinite Hilbert space of one-particle states is not truncated. Therefore, the analytic expression for the self-energy can be used to study the convergence of the energy gap between the highest occupied and the lowest unoccupied quasiparticle orbital with respect to the total number of states included in the spectral summations. The obtained asymptotic formula shows that the truncation error is dominated by a term proportional to the cutoff energy to the power -3/2, which is compatible with earlier numerical results for band gaps in real materials.

HL 84.2 Wed 17:00 P1

Defect energy levels: Hybrid density functional theory vs. many-body perturbation theory — •WEI CHEN and ALFREDO PASQUARELLO — Chaire de Simulation à l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We establish a consistent description of the thermodynamic charge transition levels of localized point defects through hybrid density functional theory and many-body perturbation theory. Three point defects are presented in this work, including a color center (a fluorine vacancy) in lithium fluoride, an oxygen interstitial in silicon oxide, and a carbon split interstitial with  $\langle 100 \rangle$ -orientation in cubic silicon carbide. The choice of the defects spans atomically localized defects in both ionic insulators and covalent semiconductors. The hybrid-functional calculations are performed using the PBE0 and the range-separated HSE functionals. The  $G_0W_0$  calculations are performed on top of PBE eigenvalues and eigenstates. We find that the total-energy difference method using (hybrid) density functionals yields remarkably compatible charge transition levels relative to the higher level  $G_0W_0$ approach, provided the electronic structures are aligned with respect to the electrostatic potential. We highlight the importance of the finitesize effect, the delocalization error, and the choice of the calculation path in the  $G_0 W_0$  scheme of the defect level calculation. Our results substantiate the need of a correct description of the band edges in the prediction of defect energy levels.

## HL 84.3 Wed 17:00 P1

**Depth-Localization of Nitrogen-Vacancy-Centers in Diamond** with Subwavelength-Accuracy — •ANDREAS HÄUSSLER and FE-DOR JELEZKO — Institut für Quantenoptik, Universität Ulm, Albert-Einstein-Allee 11, 89081 Ulm , Germany

Nitrogen-Vacancy (NV) color centers in diamond are interesting candidates for several applications, e.g. magnetic sensing in solid state. In certain cases it is crucial to know the exact position of the center below the surface.

In our work, we use a simple confocal microscope and measure both the reflected light from the surface and the emitted light of the NV to determine the depth of the color center. Suitable calibration measurements and statistical evaluation of the data can then lead to a much higher precision than the point spread function of the microscope down to nanometer accuracy.

## HL 84.4 Wed 17:00 P1

Peapods on NV-centers in diamond for quantum computing —  $\bullet$ FABIAN FRITZ<sup>1,5</sup>, CHRISTIAN SPUDAT<sup>2</sup>, LOTHAR HOUBEN<sup>3,5</sup>, Location: P1

NICOLAS WÖHRL<sup>4</sup>, CLAUS M. SCHNEIDER<sup>1,4</sup>, and CAROLA MEYER<sup>1,5</sup> <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Jülich, Germany —  $^2 {\rm Fraunhofer}$  ENAS Chemnitz, Germany —  $^3 {\rm Ernst}$  Ruska-Centre for Microscopy and Spectroscopy with Electrons, Jülich, Germany -<sup>4</sup>University Duisburg-Essen and CeNIDE, Faculty of Physics, Germany — <sup>5</sup>JARA - Fundamentals of Future Information Technologies The electron spin of an endohedral fullerene like  $N@C_{60}$  is very well shielded from the environment showing a long spin coherence time and thus resembles a good quantum bit. The read-out of an individual electron spin remains a challenge but can be achieved by coupling the spin of the N@C<sub>60</sub> to an NV-center in diamond. In order to couple several quantum bits, the  $N@C_{60}$  molecules have to be aligned in a one-dimensional chain. This can be accomplished by filling the  $N@C_{60}$ into carbon nanotubes (CNTs), forming so-called peapods. To form such a quantum register, peapods have to be fabricated and placed on diamond substrates.

We present growth of CNTs directly on a diamond surface using chemical vapor deposition (CVD). For the peapod synthesis we use solvent filling instead of vapor filling, since the N@C<sub>60</sub> fullerenes are thermally instable. Peapods are synthesized using different solvents and characterized using high-resolution transmission electron microscopy. The most promising solvent to prevent residues in the CNTs is super-critical CO<sub>2</sub> due to the small-sized molecules.

HL 84.5 Wed 17:00 P1 Magnetotransport in carbon nanotube networks functionalized with tetranuclear metal complexes — •MARLOU SLOT<sup>1,4</sup>, MICHAEL SCHNEE<sup>1,4</sup>, CLAIRE BESSON<sup>1,2,4</sup>, FABIAN FRITZ<sup>1,4</sup>, ROBERT FRIELINGHAUS<sup>1,4</sup>, LOTHAR HOUBEN<sup>1,3,4</sup>, CHRISTOPHER NAKAMOTO<sup>1,4</sup>, PAUL KÖGERLER<sup>1,2,4</sup>, CLAUS M. SCHNEIDER<sup>1,4</sup>, and CAROLA MEYER<sup>1,4</sup> — <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Jülich, Germany — <sup>2</sup>Institut für Anorganische Chemie, RWTH Aachen, Germany — <sup>3</sup>Ernst Ruska-Centre, Forschungszentrum Jülich, Germany — <sup>4</sup>JARA - Fundamentals of Future Information Technologies

Carbon nanotubes (CNTs) exhibit outstanding electronic and spin transport properties. These properties can be manipulated by chemical functionalization. We present CNT networks, grown by chemical vapor deposition, to which tetranuclear cobalt(II), manganese(II) and zinc(II) coordination complexes are attached. In contrast to commonly used van der Waals bonding, where the molecular orientation with respect to the CNT is arbitrary, we fix the angle between CNT and complex using covalent functionalization. Since the chemical route is based on carboxylate ligand exchange, oxidation of the CNTs before the functionalization is required. Raman spectroscopy is used to optimize the oxidation with respect to the desired density of carboxylate groups and the resistance of the CNT network. Magnetotransport measurements at temperatures down to 3 K show a resistance increase towards lower temperatures and a negative magnetoresistance. The underlying transport mechanism and the effect of the functionalization with magnetic complexes on the magnetoresistance are analyzed.

#### HL 84.6 Wed 17:00 P1

Quantum transport in functionalized carbon nanotubes — •MICHAEL SCHNEE<sup>1,3</sup>, ROBERT FRIELINGHAUS<sup>1,3</sup>, CLAIRE BESSON<sup>1,2,3</sup>, PAUL KÖGERLER<sup>1,2,3</sup>, CLAUS M. SCHNEIDER<sup>1,3</sup>, and CAROLA MEYER<sup>1,3</sup> — <sup>1</sup>Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Institut für Anorganische Chemie, RWTH Aachen, 52074 Aachen, Germany — <sup>3</sup>JARA - Fundamentals of Future Information Technologies

Carbon nanotubes are a promising material with regard to future nanoelectronic applications due to their exceptional mechanical and electronic properties. Moreover, the transport properties can be altered by attaching molecules to the CNTs. Thus, electronic transport experiments on functionalized CNTs can be used to study CNT-molecule interactions.

In this work we present experiments conducted on CNTs covalently functionalized with tetramanganese coordination complexes. The functionalization procedure is very versatile and manganese can be exchanged with several other metals.

The CNTs are cooled down to a temperature of T=25mK using a dilution refrigerator. First results of quantum transport experiments

on functionalized CNTs suggest a quantum dot size similar to the designed device length. This indicates that the electron wave function is only weakly disturbed and coherence is not destroyed by the covalent bonding of a small number of molecules. Therefore, quantum transport spectroscopy can be used to study the interactions between CNTs and the attached molecules.

## HL 84.7 Wed 17:00 P1

study of electrical and mechanical properties of single walled carbon nanotubes —  $\bullet$ MARYAM YOUHANNAYEE<sup>1</sup>, MATHIAS GETZLAFF<sup>1</sup>, and HOSSEIN GOLNABI<sup>2</sup> — <sup>1</sup>Heinrich Heine Universität Düsseldorf — <sup>2</sup>Sharif university of technology

In this research, using the single-band tight-binding approach and the energy dispersion relation, variation of band gap energy due to the effect of uniaxial stress on the zigzag and armchair single wall carbon nanotubes has been investigated analytically. The obtained results show that in all the zigzag carbon nanotubes, the band gap behaves linearly with increasing the uniaxial stress and one can observe a transition from semiconducting to metallic. In case of zigzag nanotubes with small diameter we have critical point which in that point critical break happens. The armchair carbon nanotubes are disable in response to the uniaxial stress and their metallic behavior is retained.

This research also investigates the electromechanical coupling in single-walled carbon nanotubes. In the model system, the extra electric charge of nanotubes is assumed to be uniformly distributed between carbon atoms. The electrostatic interactions between charged carbon atoms are calculated using the Coulomb law. It is shown that the classical electrostatics is computationally efficient. I studied a simplified electron lattice model at low charge injection levels and showed that the electromechanical actuation of SWNTs strongly depends on (N, M). N and M are the chiral index that shows different kind of nano tubes. The effects of charge injection (electron and hole), tube diameter on longitudinal, radial and torsional angle change have been examined.

#### HL 84.8 Wed 17:00 P1

**I-V characterisation of a-Si/c-Si heterojunctions** — •PATRICK THOMA, EVELYN T. BREYER, OVIDIU D. GORDAN, and DIETRICH R. T. ZAHN — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

As pure crystalline silicon solar cells have limited light absorption efficiency due to their indirect band gap requiring thick absorption layers manufactured in an energy intensive production process, research tries to find new cheaper and more efficient systems for energy harvesting. One promising approach is the use of so called heterojunction solar cells, consisting of different semiconducting material layers which have advantages like complementary absorbance of light in various wavelength regions and lower production cost. The heterojunction of amorphous and crystalline silicon combines a favorable absorption characteristic for the solar spectrum and could reduce the amount of silicon used due to overall thinner films. For sample preparation, thin layers of amorphous silicon (a-Si) were prepared by magnetron sputtering in high vacuum on HF-etched p-type crystalline silicon (c-Si). During the sputtering process deposition parameters like temperature, hydrogen flow rate and film thickness of the amorphous film were varied. Using ohmic Nickel-Chromium back and front contacts, the samples were investigated by temperature dependent I-V characterisation and measurements under illumination using a solar simulator. Especially the influence of hydrogen flow rate on the current voltage (I-V) characteristics, barrier heights and thermal activation energies are shown in relation with cell efficiencies.

## HL 84.9 Wed 17:00 P1

Electronic and optical properties of amorphous Ge nanocrystals in a crystalline Si matrix — •MORITZ LAUBSCHER<sup>1</sup>, SEBASTIAN KÜFNER<sup>1</sup>, JÜRGEN FURTHMÜLLER<sup>1</sup>, PETER KROLL<sup>2</sup>, and FRIEDHELM BECHSTEDT<sup>1</sup> — <sup>1</sup>Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — <sup>2</sup>Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas 76019, USA

Embedded Ge nanocrystals have been discussed as promising elements for novel optoelectronic devices, because of their luminescence and charge rentention properties. The low dimensionality, together with the heterojunctions formed by the nanocrystals and the matrices, lead to (unique) quantum-confined electronic states and therefore new tunable electronic and optical properties. In contrast to the well investigated embedded c-NC, amorphous Ge nanocrystalls have not been studied in an *ab-initio* framework. Usually, Ge NCs show quantum confinment effects, e.g. size-depended photoluminescence. The Ge/Si interfaces most likely build a type II heterostructure. It is not known how amorphousness together with quantum confinment and the interface between NCs and matrices effect electronic structure and therefore optical properties. In this study we use a algorithm analogue to the WWW-algorithm in order to generate embedded amorphous nanocrystals and the density functional theory with the Tran-Blaha approximation to simulate the electronic and optical properties near the fundamental gap with quasiparticle corrections. We discuss optical properties and possible photoluminescence by calculating optical dipole matrix elements.

HL 84.10 Wed 17:00 P1 Comparison of melting properties reproduced by the MOD Tersoff potential in diamond silicon structures with experimental values. — •ROBERT KÖNIG, VLADIMIR LIPP, DMITRIY S. IVANOV, and MARTIN E. GARCIA — Universität Kassel, Institut für Physik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Abstract

Inspite of being one of the most widely used interatomic potentials for silicon, the Tersoff potential showed some discrepancies for the description of the melting properties for diamond silicon. In order to clear this issue Sakai et al. improved the Tersoff potential through changes in the angular dependent term. The improved potential was named the MOD Tersoff potential. Using classical Molecular Dynamics the properties of the MOD Tersoff potential at the melting point were computed in two ways. First the equilibrium melting temperature was determined from a sequence of liquid-crystal coexistence simulation performed at different pressures. In the second part, other properties like the volume of melting and the enthalpie of melting were found from another sequence of constant pressure and constant temperature simulations where the interatomic distance and the energy per atom were computed as a function of temperature. The results showed good agreement with their experimental values published in literature.

#### HL 84.11 Wed 17:00 P1

Cathodoluminescence and Electron Beam Induced Current Study on Grain Boundaries in Silicon — •MARKUS NACKE<sup>1</sup>, MATTHIAS ALLARDT<sup>1</sup>, PAUL CHEKHONIN<sup>2</sup>, ELLEN HIECKMANN<sup>1</sup>, and JÖRG WEBER<sup>1</sup> — <sup>1</sup>TU Dresden, IAP/ Halbleiterphysik — <sup>2</sup>TU Dresden, ISP/ Metallphysik

Temperature dependent cathodoluminescence (CL) and room temperature electron beam induced current (EBIC) measurements have been used to investigate the optical behaviour and electrical activity of grain boundaries (GBs) in silicon. Electron backscatter diffraction (EBSD) was applied for a comprehensive characterization of the structural properties of the GBs including the misorientationaxis and -angle as well as the crystallographic orientation of the GB plane. It was found that the panchromatic CL contrast of  $\Sigma 3$  large-angle GBs depends strongly from the hkl-type of the GB plane. The results are in agreement with EBIC investigations on coherent and incoherent twins in Si. D1 emission (0.812 eV) was detected at a small-angle GB (SA-GB). Other D-lines were not observed. Mono- and pan-CL investigations performed in the temperature range from 4.5K to 50K revealed a complex CL contrast behaviour of the SA-GB. Cross-correlation (CC-) EBSD was applied to analyze the relationship between the strain field of the SA-GB and the spatial D1 emission distribution. CC-EBSD results indicate that the crystal lattice is locally expanded at the SA-GB.

## HL 84.12 Wed 17:00 P1

Electrical characterization of femtosecond laser sulfur doped silicon — •ARNE AHRENS<sup>1</sup>, PHILIPP SARING<sup>1</sup>, ANNA LENA BAUMANN<sup>2</sup>, STEFAN KONTERMANN<sup>2</sup>, WOLFGANG SCHADE<sup>2</sup>, and MICHAEL SEIBT<sup>1</sup> — <sup>1</sup>IV.Physikalisches Institut, Georg-August Universität Göttingen, Friedrich Hund Platz 1, 37077 Göttingen, Germany — <sup>2</sup>Frauenhofer Heinrich Hertz Institute, Am Stollen 19B, 38640 Gosslar, Germany

Femtosecond (fs) laser pulse irradiation in sulfur hexaflouride atmosphere is a versatile tool to modify optical and electrical properties of silicon. Structuring of the surface and sulfur doping beyond the solubility limit (hyperdoping) enhance optical absorption in the subbandgap and in the visible range which is attributed to surface structuring and the introduction of deep levels, respectively. Especially the sub-bandgap absorption makes such material a promising candidate for intermediate band solar cell applications, especially if impurity bands form due to a Mott transition [1]. In case of p-type silicon substrates, sulfur hyperdoping also leads to the formation of a buried pn-junction which has recently been studied by means of cross-section transmission electron microscopy (TEM) and electron-beam induced current (EBIC) [2] as well as capacitance-voltage (CV) and SIMS measurements [3]. In this work, we apply EBIC, temperature-dependent CV- and deep-level transient spectroscopy (DLTS) to study deep levels which are introduced by the irradiation with fs laser pulses accompanied by careful TEM analyses. [1] M. Winkler et al., Phys. Rev. Lett. 106, 178701 (2011). [2] P. Saring et al., Appl. Phys. Lett. 102, 202104 (2013) [3] K.-M. Guenther et al., Appl. Phys. Lett. 102, 202104 (2013)

#### HL 84.13 Wed 17:00 P1

How to explain laser induced Si->SiO2 electron injection at front and rear interfaces of a Si membrane? — •PER-CHRISTIAN HEISEL<sup>1</sup>, WOLFGANG PAA<sup>1</sup>, and HERBERT STAFAST<sup>1,2</sup> — <sup>1</sup>Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena — <sup>2</sup>Faculty of Physics & Astronomy, Max-Wien-Platz 1, 07743 Jena

Electrical field induced second harmonic generation (EFISH) is well known for Si/SiO2 interfaces and typically measured in reflection [1]. EFISH in transmission was first shown with an external field applied to a 100 microns thick MOS structure [2]. The first comparison of EFISH in reflection and transmission was shown recently [3,4] using a 10 microns thick, naturally oxidized Si membrane. The rear EFISH signal (transmission) rises much faster than the front signal (reflection) and yields a larger steady state value. These findings essentially originate from differences in the laser induced electron injection from Si to SiO2. Their explanation is approached by different models like e. g. the image force model.

[1] G. Lüpke, Surf. Sci. Rep. 35, 77 (1999)

[2] O. A. Aktisipetrov et al., Opt. Lett. 19, 1450 (1994)

[3] G. P. Nyamuda, PhD thesis, University Stellenbosch, South Africa (2010)

[4] G. P. Nyamuda et al., Appl. Phys. B 104, 735 (2011)

#### HL 84.14 Wed 17:00 P1

**Coherent Transport in GaAs/InAs Core/Shell Nanowires** — •PATRICK ZELLEKENS<sup>1,2</sup>, FABIAN HAAS<sup>1,2</sup>, TOBIAS WENZ<sup>1,2</sup>, NA-TALIA DEMARINA<sup>1,2</sup>, TORSTEN RIEGER<sup>1,2</sup>, MIHAIL LEPSA<sup>1,2</sup>, DETLEV GRÜTZMACHER<sup>1,2</sup>, HANS LÜTH<sup>1,2</sup>, and THOMAS SCHÄPERS<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institute - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>JARA - Fundamentals of Future Information Technology

GaAs/InAs core/shell nanowires are very interesting objects for studying magnetic flux dependent quantum transport phenomena, due to the fact that the low bandgap InAs shell forms a cylindrical tube-like conductor around the high bandgap GaAs core. This allows the emergence of phase coherent transport phenomena, i.e. (h/e) flux-periodic conductance oscillations. In this contribution, we present magnetotransport measurements of GaAs/InAs core/shell nanowires at various temperatures in a magnetic field applied parallel to the wire axis. The magneto conductance of the core/shell nanowires revealed pronounced h/e-periodic oscillations, which can be attributed to electronic transport via angular momentum states. In a more detailed analysis higher harmonic h/2e periodic oscillations were also resolved. In nanowires comprising a small core diameter of 70nm the h/e oscillations are visible at temperatures up to 50 K, indicating a large energetic separation of successive angular momentum states. These findings are supported by gate-dependent universal conductance fluctuation measurements, which show thermal stability of phase coherent transport up to 40 K.

## HL 84.15 Wed 17:00 P1

Properties of exciton-polariton gap-solitons in a twodimensional lattice —  $\bullet$ EDGAR CERDA-MENDEZ<sup>1</sup>, DIMITRYI KRIZHANOVSKII<sup>2</sup>, SERGEI GAVRILOV<sup>3</sup>, KLAUS BIERMANN<sup>1</sup>, MAURICE S. SKOLNICK<sup>2</sup>, and PAULO SANTOS<sup>1</sup> — <sup>1</sup>Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — <sup>2</sup>University of Sheffield, Sheffield, United Kingdom — <sup>3</sup>Institute of Solid State Physics, Chernogolovka, Russia

Exciton-polaritons are bosonic quasi-particles that result from the strong coupling of photons and quantum well excitons in a semiconductor microcavity (MC). While the small mass arising from the photonic component allows polaritons to form condensates at low densities and high temperatures, the repulsive excitonic interactions provide a strong nonlinearity. The periodic spatial modulation of the MC creates an artificial band structure with energy gaps and negative dispersion. Due to the nonlinearity, spatially self-localized polariton states, known as gap solitons (GSs), may appear within the energy gaps when the kinetic energy contribution due to localization of polaritons with a negative mass compensates their repulsive interaction energy. In this work, we show that the properties of polariton condensate GSs are well described by a simple variational approach to solve the Gross-Pitaevskii equation. The GSs form in an (Al,Ga)As-based MC where a 2D tunable lattice is created by surface acoustic waves. We calculated the metastable states in the square lattice. The model predicts the observed real and k-space profiles of the GS as well as the dependence of its coherence length and optical threshold power with the lattice amplitude.

HL 84.16 Wed 17:00 P1

Growth of GaAs nanowires on GaAs (111)B substrates induced by focused ion beam — •RÜDIGER SCHOTT, SVEN SCHOLZ, DIRK REUTER, ARNE LUDWIG, and ANDREAS D. WIECK — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor nanowires (NWs) are used as building blocks for a new generation of advanced devices intended for different applications in the field of nanoelectronics, nanophotonics and nanomechanics. NWs are near one-dimensional structures that typically have a high lengthto-width ratio. This is the base of samples fascinating structural properties. Heterostructures of highly lattice mismatched materials can be combined without dislocations and the growth metastable phases, unattainable in bulk materials like wurtzite GaAs, can be made. We present focused ion beam (FIB) induced molecular beam epitaxy (MBE) grown single GaAs nanowires on GaAs (111)B substrates from site selectively deposited Au seeds. Structural and optical properties of the nanowires are investigated by secondary electron microscopy (SEM), transmission electron microscopy (TEM) and photoluminescence spectroscopy (PL).

## HL 84.17 Wed 17:00 P1

Epitaxial growth of heterostructures on GaAs (111)A and GaAs (111)B substrates — •JULIAN RITZMANN, ARNE LUD-WIG, RÜDIGER SCHOTT, DIRK REUTER, and ANDREAS D. WIECK — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum, Germany

Heterostructures on (111)-oriented GaAs substrates are known for possibly high light emitting efficiency and tunable electron spin lifetimes by suppressing the Dyakonov-Perel relaxation. This offers a wide range for new and unique devices in the field of spintronics and -optics. The growth by molecular beam epitaxy on these surfaces is however rather challenging and only a limited range of growth parameters leads to structures of high crystal quality.

In this work we present the capabilities of MBE-grown AlGaAs and GaAs layers on (111)A and (111)B GaAs substrates without miscut. The samples exhibit reduced surface roughness and good electrical properties shown by atomic force and scanning electron microscopy and van-der-Pauw Hall measurements.

#### HL 84.18 Wed 17:00 P1

Photo-modulated reflection spectroscopy of Ga(AsBi) bulk and quantum well structures — •JAN KUHNERT, PETER LUDEWIG, KERSTIN VOLZ, and SANGAM CHATTERJEE — Philipps-Universität Marburg, Marburg, Germany

Bismuth-containing structures based on GaAs are promising candidates for semiconductor lasers operating at telecom wavelength. By an incorporation of about 10% bismuth, this desired wavelength of 1550nm is reached. In this system the reduction of band gap is due to shifting of the valence bands rather than the conduction band. Besides the influence on the band gap, the spin orbit coupling is increased and the gap between the valence bands is increased[1]. This way, losses due to auger processes are reduced and high temperature efficiency is increased.To quantify the influence of bismuth concentration, we investigated multiple Ga(AsBi)/GaAs bulk samples with different Bi concentrations by room temperature photo-modulated reflection spectroscopy. In addition, to characterize confinement effects, a set of multi quantum well structures is investigated using the same technique. [1] Appl. Phys. Lett. 91, 051909, (2007)

#### HL 84.19 Wed 17:00 P1

**Temperature-dependent external quantum efficiency of Ga(AsBi)** — •PHILIPP VLACIL, NILS ROSEMANN, PETER LUDEWIG, KERSTIN VOLZ, and SANGAM CHATTERJEE — Philipps-Universität Marburg, Marburg, Germany

Dilute bismuth-containing alloys of GaAs have recently gained a lot of interest due to the large band gap reduction of about 60meV per percentage of bismuth. This large bowing shifts the Band gap of the alloy

towards the telecom wavelength for concentrations of about 10%. This band gap shift is a consequence of modifications to the valence bands rather than the conduction bands, which are shifted, e.g. when In or N are incorporated. Additionally, the spin orbit coupling is increased and the shift of the split-of valence band is significantly increased[1], inhibiting hole-related Auger recombination processes. Nevertheless, the rather large covalent radius of bismuth induces significant disorder effects in such alloys. To quantify these, we investigated two sets of Ga(AsBi)/GaAs bulk and multiple quantum well (MQW) samples with different Bi concentrations by temperature-dependent absolute photoluminescence spectroscopy using an integrating sphere mounted inside a closed-cycle cryostat. The temperature dependence of the luminescence is used to quantify disorder. [1] Appl. Phys. Lett. 91, 051909, (2007)

HL 84.20 Wed 17:00 P1 The influence of growth parameters on the phase composition and defect structure of InAs nanowires — •ANTON DAVYDOK<sup>1,2</sup>, ANDREAS BIERMANNS-FÖTH<sup>1</sup>, EMMANOUL DIMAKIS<sup>3,4</sup>, LUTZ GEELHAAR<sup>3</sup>, and ULLRICH PIETSCH<sup>1</sup> — <sup>1</sup>Universität Siegen, Siegen, Germany — <sup>2</sup>Im2np, Marseille, France — <sup>3</sup>Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — <sup>4</sup>Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

We presented the results of X-ray investigation of MBE grown InAs nanowires (NWs) onto silicon (111) substrate. It was found that InAs NWs preferentially grow in wurtzite phase but may contain a large number of stacking faults (SF). The aim of this work was to investigate the influence of various growth parameters as temperature, In-flux, V/III ratio etc.) on the structural phase composition. The density of SF has been evaluated from the FWHM of the (10i5) wurtzite Bragg reflection which is particularly sensitive to SF inclusions, followed by numerical simulations using a model of a statistical distribution of SF in an ensemble of many nanowires. It has been found that nearly independent from the choice of growth parameters a low SF density is found in the initial phase of NW growth. With increasing growth time the increase of SF density can be described by a function SF-den=A\*exp(-L/d)+m, with A=0.37, d=-752 and m=0.41. The SF density increases fast in the beginning but saturates for longer growth time.

 $\label{eq:HL-84.21} \begin{array}{ccc} \mathrm{HL} \ 84.21 & \mathrm{Wed} \ 17:00 & \mathrm{P1} \\ \\ \mathbf{Self-assembled} & \mathbf{growth} \ \ \mathbf{of} \ \ \mathbf{InxGa1-xAs} \ \ \mathbf{quantum} \ \ \mathbf{dots} \ \ \mathbf{on} \end{array}$ 

**GaP by gas-source molecular-beam epitaxy** — •SHABNAM DADGOSTAR<sup>1</sup>, FARIBA HATAMI<sup>1</sup>, W. TED MASSELINK<sup>1</sup>, JAN SCHMIDTBAUER<sup>2</sup>, and TORSTEN BOECK<sup>2</sup> — <sup>1</sup>Departmant of physics, Humboldt university of Berlin. Newtonstr. 15, 12489 Berlin. Germany. — <sup>2</sup>Leibniz- Institute für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The InGaAs/GaP heterosystem is expected to be type I, suggesting its use for light emission. We have used gas-source molecular-beam epitaxy to grow InxGa1-xAs (x=0.3, 0.5) quantum dots on GaP (100) substrates; the lattice mismatch is 6.0 and 7.4 %, x=0.3 and x=0.5. For a coverage of 2 monolayers of In0.3Ga0.7As deposited at 0.4 ML/s, however, AFM indicates the formation of high density of In0.3Ga0.7As quantum dots. Their density is 1.2 e11 cm-2, with average diameter and height of 12.5 nm and 2.5 nm, respectively. For In0.5Ga0.5As deposited under the same conditions, however, AFM measurements show evolution of large islands with diameter of 95 nm and height of 20 nm. The critical thickness for transition from two-dimensional to three dimensional growth was determined by AFM results and it was found less than 1.5 and 1.3 monolayers for In0.3Ga0.7As and In0.5Ga0.5As respectively.

Structural properties of AlGaP films on GaP grown by gassource molecular-beam empitaxy. — •SHABNAM DADGOSTAR<sup>1</sup>, EMAD HAMEED HUSSEIN<sup>1</sup>, W. TED MASSELINK<sup>1</sup>, FARIBA HATAMI<sup>1</sup>, JAN SCHMIDTBAUER<sup>2</sup>, and TORSTEN BOECK<sup>2</sup> — <sup>1</sup>Departmant of physics, Humboldt university of Berlin. Newtonstr. 15, 12489 Berlin. Germany. — <sup>2</sup>Leibniz- Institute für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

High-Q photonic crystal cavities with working range in visible wavelengths can be realized based on GaP membranes. Such membranes can be prepared as a single crystal using gas-source molecular-beam epitaxy with a sacrificial layer of AlGaP. High quality factor of photonic crystal cavity is limited by crystal quality of GaP membrane which depends on AlGaP sacrificial layer crystal quality. We have studied the effects of growth temperature and PH3 flux on the crystal quality of AlGaP layer. For our applications we used AlGaP structures with thickness of 1.0  $\mu$ m and Al content of 85%. Both high-resolution x-ray diffraction and AFM measurements indicate that dislocation and oval-defects are minimized for growth temperature of 4900C and PH3 flux of 2.7 sccm.

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