Time: Wednesday 9:30–13:00

HL 36.1 Wed 9:30 H14 Univers

**Optical studies of P-, Al-, Ga- and As-doped Ge** – •MATTHIAS ALLARDT<sup>1</sup>, VLADIMIR KOLKOVSKY<sup>1</sup>, PAUL CLAUWS<sup>2</sup>, and JÖRG WEBER<sup>1</sup> – <sup>1</sup>Technische Universität Dresden, 01062 Dresden, Germany – <sup>2</sup>Ghent University, 9000 Gent, Belgium

In the present work (P, As, Ga, Al) doped Ge was used to study the shallow impurities in this elemental semiconductor. Photoluminescence measurements at 4.2 K reveal for the first time the Al bound exciton observed in the LA region. The intensity of the Al bound exciton is consistent with the Al content inside the sample. Our results can be also correlated with the IR absorption measurements performed at low temperatures. We verify that Al is the dominant impurity in Al-doped Ge and the observed bound exciton signal is unambiguously related to Al.

 $\rm HL \ 36.2 \quad Wed \ 9{:}45 \quad H14$ 

Intrinsic and extrinsic diffusion of indium in germanium — •RENÉ KUBE<sup>1</sup>, HARTMUT BRACHT<sup>1</sup>, ALEXANDER CHRONEOS<sup>2</sup>, MATTHIAS POSSELT<sup>3</sup>, and BERND SCHMIDT<sup>3</sup> — <sup>1</sup>Institut für Material-physik, WWU Münster, Germany — <sup>2</sup>Department of Materials, Imperial College, London, UK — <sup>3</sup>Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

Diffusion experiments with indium (In) in germanium (Ge) were performed in the temperature range between 550 and 900°C. Intrinsic and extrinsic doping levels were achieved by utilizing various implantation doses. Indium concentration profiles were recorded by means of secondary ion mass spectrometry and spreading resistance profiling. The observed concentration independent diffusion profiles are accurately described on the basis of the vacancy mechanism with a singly negatively charged mobile In-vacancy complex. In accord with the experiment, the diffusion model predicts an effective In diffusion coefficient under extrinsic conditions that is a factor of two higher than under intrinsic conditions. The temperature dependence of intrinsic In diffusion yields an activation enthalpy of 3.51 eV and confirms earlier results of Dorner et al. [Z. Metallk. 7, 325 (1982)]. The value clearly exceeds the activation enthalpy of Ge self-diffusion and indicates that the attractive interaction between In and a vacancy does not extend to third nearest neighbor sites which confirms recent theoretical calculations.

# HL 36.3 Wed 10:00 H14

The impact of interstitials on diffusion in germanium under proton irradiation — •SEBASTIAN SCHNEIDER<sup>1</sup>, HARTMUT BRACHT<sup>1</sup>, JAN KLUG<sup>2</sup>, JOHN LUNDSGAARD HANSEN<sup>3</sup>, ARNE NY-LANDSTED LARSEN<sup>3</sup>, EUGENE HALLER<sup>4</sup>, DOMINIQUE BOUGEARD<sup>5</sup>, MATTHIAS POSSELT<sup>6</sup>, and CLEMENS WÜNDISCH<sup>6</sup> — <sup>1</sup>Institut für Materialphysik, WWU Münster, Germany — <sup>2</sup>Ruhr-Universiät, Bochum, Germany — <sup>3</sup>Department of Physics and Astronomy, University of Aarhus, Denmark — <sup>4</sup>MS and E Dept. University of California, Berkeley, U.S.A — <sup>5</sup>Walter-Schottky-Institut, TU München, Germany — <sup>6</sup>FZ Dresden-Rossendorf, Dresden, Germany

Experiments on the influence of 2.5 MeV proton irradiation on selfand dopant diffusion in germanium (Ge) were performed at 600 and  $570^{\circ}$ C, respectively. Ge isotope heterostructures consisting of 20 layers were used for the self-diffusion study. Ge with boron (B) doped multilayers and samples implanted with phosphorus (P) were utilized for the investigation of irradiation mediated dopant diffusion. Selfdiffusion under irradiation reveals an unusual homogenous broadening of the isotope structure. This behaviour and the enhanced diffusion of B and retarded diffusion of P under irradiation demonstrates that an interstitial-mediated diffusion process dominates in Ge under irradiation. This discovery establishes new ways to suppress vacancymediated diffusion in Ge and to solve the donor deactivation problem that limits Ge-based nanoelectronics.

HL 36.4 Wed 10:15 H14 Influence of electronic energy deposition on structural modification of SHI irradiated amorphous Ge layers — •TOBIAS STEINBACH<sup>1</sup>, WERNER WESCH<sup>1</sup>, CLAUDIA S. SCHNOHR<sup>1</sup>, LEANDRO L. ARAUJO<sup>2</sup>, RAQUEL GIULIAN<sup>2</sup>, DAVID J. SPROUSTER<sup>2</sup>, and MARK C. RIDGWAY<sup>2</sup> — <sup>1</sup>Institute of Solid State Physics, Friedrich Schiller University Jena — <sup>2</sup>Department of Electronic Materials Engineering, Australian National University, Canberra

During SHI irradiation of amorphous Ge a strong swelling of the amorphous layer accompanied by an enhanced plastic flow process was observed in previous studies. To study the effect of high electronic energy deposition  $\epsilon_e$  on amorphous Ge layers in more detail the samples were irradiated with 185 and 89 MeV Au ions with different incident angles. In order to quantify the swelling and the plastic flow process, a grid of Au was evaporated on the sample surface and one half of the sample was masked to distinguish the irradiated from the unirradiated reference. We demonstrate for all used irradiation conditions that a strong swelling of the irradiated areas can be observed, which depends linearly on the ion fluence as well as on  $\epsilon_e$ . XSEM revealed the transformation of the initially homogeneous amorphous Ge layer into a sponge-like porous structure with irregularly shaped voids thus establishing that swelling was a consequence of void formation. Moreover, an electronic energy deposition threshold has been estimated, at which the swelling, i.e. the formation of voids, begins. In addition, the ion beam induced plastic flow process is directly apparent in the XSEM and will be discussed as a function of the ion fluence and  $\epsilon_e$ .

## HL 36.5 Wed 10:30 H14

First Principles Study of the Oxide at the Ge-GeO<sub>2</sub> Interface —  $\bullet$ JAN FELIX BINDER, PETER BROQVIST, and ALFREDO PASQUARELLO — Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Theoretical Physics, CH-1015, Switzerland

As Si-based metal-oxide-semiconductor devices are approaching their technological and physical limits due to aggressive scaling, the search for new material solutions intensifies. Germanium shows high electron and hole mobilities together with a small electronic band gap, and is seriously being considered as a viable alternative to silicon. However, current stateof-the-art germanium-insulator interfaces show excessively high defect densities compared to conventional silicon/insulator interfaces. Hence, the characterization of both the structural and electronic properties of the  $Ge/GeO_2$  interface is highly relevant. We study germanium suboxides within a density functional approach focusing on their energetic, atomic, and electronic properties. First, we calculate penalty energies of germanium suboxides, and find significantly smaller values than for silicon. This supports a higher concentration of suboxides at  $\mathrm{Ge}/\mathrm{GeO}_2$  interfaces. Second, we generate a morphous models of GeO and  $GeO_2$  through ab initio molecular dynamics and study their structural and electronic properties. The analysis of the electronic structure of GeO reveals the occurrence of suboxide states in the lower part of the band gap of  $GeO_2$  consistent with several experimental observations at  $Ge/GeO_x$  interfaces.

# HL 36.6 Wed 10:45 H14

**Transient optical gain in Germanium quantum wells** — •SANGAM CHATTERJEE<sup>1</sup>, CHRISTOPH LANGE<sup>1</sup>, NIKO S. KÖSTER<sup>1</sup>, MARTIN SCHÄFER<sup>1</sup>, MACKILLO KIRA<sup>1</sup>, STEPHAN W. KOCH<sup>1</sup>, DANIEL CHRASTINA<sup>2</sup>, GIOVANNI ISELLA<sup>2</sup>, HANS VON KÄNEL<sup>2</sup>, and HANS SIGG<sup>3</sup> — <sup>1</sup>Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D 35032 Marburg, Germany — <sup>2</sup>CNISM and L-NESS, Dipartimento di Fisica del Politecnico di Milano, Polo di Como, via Anzani 42, I-22100 Como, Italy — <sup>3</sup>Laboratory for Micro and Nanotecnology, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

One of today's most-sought goals in semiconductor technology is the monolithic integration of microelectronics and photonics on Si. Optical gain is, in general, not expected for Si and Ge or its alloys due to the indirect nature of the band gap in this material system. Here, we show that Ge/SiGe QWs show transient optical gain and may thus be used as an optically-pumped amplifier at room temperature [1]. Further, the nonequilibrium effects which govern the relaxation dynamics of the optically injected carrier distributions in this material were observed and analyzed using a microscopic many-body theory. Strong non-equilibrium gin was obtained on a sub-100 fs time scale. Long-lived gain arising from  $\Gamma$ -point transitions is overcompensated by a process bearing the character of free carrier absorption.

[1] C. Lange et al., Phys. Rev. B 79, 201306(R) (2009)

# 15 Min. Coffee Break

## HL 36.7 Wed 11:15 H14

Identification of localized states on Si/SiGe quantum dots by means of ESR — •F. Lipps, F. Pezzoli, M. Stoffel, C. DENEKE, J. THOMAS, A. RASTELLI, V. KATAEV, O. G. SCHMIDT, and B. BÜCHNER — Leibniz Institute for Solid State and Materials Research IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany We performed electron spin resonance (ESR) measurements at 9.56 GHz on a series of heterostructures containing Si/SiGe quantum dots. The samples were characterized by means of transmission electron microscopy, atomic force microscopy and photoluminescence. Two distinct ESR peaks associated with electrons confined on the quantum dots were observed, characterized by different g-factors, anisotropies of the linewidth and g-factors as well as sensitivity to the illumination with sub-band gap light. Based on the structural information the electronic structure of the studied heterostructures was calculated. The single band calculations allow us to attribute the observed ESR peaks to the s- and p-like-electronic states on the quantum dots.

#### HL 36.8 Wed 11:30 H14

Towards efficient Silicon-based light sources using tailored photonic materials — •NORMAN HAUKE<sup>1</sup>, THOMAS ZABEL<sup>1</sup>, DOMINIQUE BOUGEARD<sup>1</sup>, GERHARD ABSTREITER<sup>1</sup>, YASUHIKO ARAKAWA<sup>2</sup>, and JONATHAN FINLEY<sup>1</sup> — <sup>1</sup>Walter Schottky Institut, Garching — <sup>2</sup>University of Tokyo, Japan

We present optical investigations of two-dimensional (2D) silicon (Si) photonic crystal (PhC) defect nanocavities. Temperature dependent spatially resolved  $\mu$ -photoluminescence ( $\mu$ PL) measurements in the range 20K-300K show that the emission in the cavity mode stems mainly from the bulk Si phonon satellites. Unlike in bulk and nanopatterned Si, emission from the cavity can be observed up to room-temperature. Moreover, quantitative analysis of the temperature stability spectrally in- and out-of-resonance with the cavity mode suggests that the enhanced emission at the cavity reflects enhanced internal quantum efficiency due to the Purcell-effect.

We also present temperature dependent  $\mu$ PL studies on 2D Si PhC slabs with epitaxial grown high-density  $(10^{11}cm^{-2})$  Ge-islands acting as an internal light source. We demonstrate strong enhancement of the quantum dot emission at cavity mode resonance and interpret our findings as being due to a combination of spatial redistribution of the emitted light and Purcell-effect. We also present first time-resolved  $\mu$ PL measurements that compare the radiative lifetime when detecting on the PhC with the unpatterned region of our devices.

Supported financially by the DFG via NIM, TUM IGSSE and TUM IAS.

## HL 36.9 Wed 11:45 H14

**Electrically active dopant profiles in individual silicon nanowires** — •PRATYUSH DAS KANUNGO<sup>1</sup>, XIN OU<sup>1,2</sup>, REINHARD KÖGLER<sup>2</sup>, PETER WERNER<sup>1</sup>, ULRICH GÖSELE<sup>1</sup>, and WOLFGANG SKORUPA<sup>2</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, Halle D-06120, Germany — <sup>2</sup>Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf e.V., P.O. Box 510119, 01314 Dresden, Germany

This contribution will be presented as Poster HL 31.47.

# HL 36.10 Wed 12:00 H14

Influence of oxide layer thickness on thermal properties of single silicon nanowires: a Raman study — •ASMUS VIERCK, SE-VAK KHACHADORIAN, JANINA MAULTZSCH, and CHRISTIAN THOMSEN — Institut für Festkörperphysik, TU-Berlin, EW 5-4, Hardenbergstr. 36, 10623 Berlin, Germany

The Raman spectra of single silicon nanowires (SiNWs) varying SiO<sub>2</sub> layer thickness were studied as a function of laser excitation power using combined atomic force microscopy (AFM) and Raman spectroscopy. Since silicon nanowires grown by chemical vapour deposition (CVD) are inevitably oxidized during fabrication, a modification in shape and size of the crystalline core can be observed, dependent on oxidation time. To determine the impact of different oxide shells on the silicon core properties, we used Raman spectroscopy to study possible alterations in phonon confinement of samples oxidized for different durations. By separating the SiNWs from their original silicon substrate, we were able to compare the spectra of single NWs with distinct width, determined by AFM. While varying the incident laser power we investigated the downshift of the transverse optical phonon in different oxidized NWs as compared to that of bulk silicon.

HL 36.11 Wed 12:15 H14

Isotope Effect on the Spin Resonance of Boron in Silicon — •ANDRE R. STEGNER<sup>1</sup>, HIROYUKI TEZUKA<sup>2</sup>, TILL ANDLAUER<sup>1</sup>, CHRISTOPH PELLINGER<sup>1</sup>, KOHEI M. ITOH<sup>2</sup>, MARTIN STUTZMANN<sup>1</sup>, and MARTIN S. BRANDT<sup>1</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — <sup>2</sup>School of Fundamental Science and Technology, Keio University, Yokohama 223-8522, Japan

The fourfold degeneracy of the Boron acceptor ground state in silicon, which is easily lifted by any symmetry breaking perturbation, allows for a strong inhomogeneous broadening of the B-related electron paramagnetic resonance (EPR) lines, e.g. by randomly distributed, defectinduced local strain. In previous studies a number of fundamental questions concerning the line shape, the magnitude of the residual broadening, and the substructure of the B resonances have remained unsolved. We show that local fluctuations of the valence band edge due to the presence of different Si isotopes in the vicinity of the B acceptors can quantitatively account for all inhomogeneous broadening effects in high purity Si with a natural isotope composition. A comparison of our calculations with previous work investigating the B acceptor ground state in the absence of an external magnetic field, provides an independent verification of the energy offsets between the valence bands of  $^{28}\mathrm{Si},\,^{29}\mathrm{Si},\,\mathrm{and}\,\,^{30}\mathrm{Si}.$  Moreover, our calculations show that the isotopic perturbation also leads to a shift in the g-value of different B-related resonance lines, which could be verified in our experiments.

#### HL 36.12 Wed 12:30 H14

A theoretical study of hyperfine parameters in amorphous silicon — •GERNOT PFANNER, CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Department for Computational Material Design, Max-Planck-Institute for Iron Research, Max-Planck-Strasse 1, D-40237 Düsseldorf

Thin-film silicon solar cells are considered as low-cost alternatives to bulk crystalline silicon (c-Si) solar cells. A disadvantage of these devices is that their efficiency is severely limited by defects. The nature of the so-called 'Staebler-Wronski' effect, i.e. light-induced metastable changes in the properties of hydrogenated amorphous silicon (a-Si:H), is not yet fully understood and remains challenging. In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling bond. However, the interpretation of the EPR spectrum requires comparison to theoretical calculations. Here, we focus on the hyperfine coupling of the unpaired electron to the nuclear spins. We present ab-initio calculations for a variety of dangling bond models in a-Si:H and consider the results in the light of systematic investigations for the c-Si dangling bond. We show that structural disorder in a-Si:H significantly modifies the trends found for c-Si and discuss whether the model Hamiltonians presently used to extract hyperfine parameters from EPR spectra can capture all relevant effects.

#### HL 36.13 Wed 12:45 H14

Solid-phase crystallization of amorphous silicon films by insitu postannealing using RPCVD — •OLIVER SKIBITZKI, YUJI YAMAMOTO, KLAUS KÖPKE, ANDREAS SCHUBERT, GÜNTER WEID-NER, BERND HEINEMANN, and BERND TILLACK — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Solid-phase crystallization of amorphous Silicon (a-Si) layer by in-situ postannealing using a single wafer Reduced Pressure Chemical Vapor Deposition (RPCVD) system was investigated for next generation high performance SiGe:C HBTs. The a-Si layers were deposited using H<sub>2</sub>- $Si_2H_6$  gas mixture on  $SiO_2/Si_3N_4$  patterned wafers. As-doped a-Si and non-doped a-Si were studied for emitter and base applications, respectively. After deposition process, epitaxial Si and a-Si were deposited on Si and on  $\mathrm{SiO}_2/\mathrm{Si}_3\mathrm{N}_4$  mask, correspondingly. By in-situ postannealing at 700 to 1000°C, the a-Si part was crystallized and polycrystalline Si was formed. Near the sidewall of the window, the a-Si was crystallized epitaxially. At higher postannealing temperatures, the grain size of crystallized poly-Si and the epitaxial domain near the sidewall became larger. Otherwise, by annealing at 575°C, direct polycrystalline formation from a-Si seems to be suppressed and the epitaxial domain near the sidewall grew with increasing annealing time. For both 700-1000°C and 575°C annealing conditions, the crystallization is inhibited if As concentration in a-Si layer raises. One possible explanation could be that the migration mobility of Si atoms during crystallization is reduced by As. These results may offer new process integration concepts for further SiGe:C HBT performance improvement.