HL 54: Si/Ge

Time: Friday 10:30–15:00 Location: EW 202

HL 54.1 Fri 10:30 EW 202

Defect Formation Energies without the Band-Gap Problem: Combining DFT and *GW* for the Silicon Self-Interstitial — •Patrick Rinke[1,2], Anderson Janotti[1], Chris G. Van de Walle[1], and Matthias Scheffler[1,2] — [1]University of California at Santa Barbara, CA 93106 — [2]Fritz-Haber-Institut der MPG, Berlin

For the self-interstitial in silicon, a defect of high technological relevance, density functional theory (DFT) in the widely applied local-density approximation (LDA) underestimates the formation energies of different configurations in the neutral charge state by about 1.5 eV compared to diffusion Monte Carlo (DMC) calculations [1,2]. We attribute this to artificial self-interaction and the absence of the derivative discontinuity in the exchange-correlation potential in the LDA that give rise to the band-gap problem. Here we present a new formalism that combines LDA with quasiparticle energy calculations in the G_0W_0 approximation to overcome these deficiencies. The formation of the neutral defect is expressed as successive charging of its 2+ charge state, for which the defect level is unoccupied. This allows us to decompose the formation energy into a lattice (LDA) and an electron addition part (G_0W_0) [3]. The G_0W_0 corrections increase the LDA formation energy of the neutral state by ∼1.1 eV. Moreover, the G_0W_0-corrected charge transition levels, which are also readily available, agree well with recent measurements [4]. [1] E. R. Batista *et al. Phys. Rev. B* **74**, 121102(R) (2006), [2] W.-K. Leung *et al. Phys. Rev. Lett.* **83**, 2351 (1999), [3] M. Hedström *et al. Phys. Rev. Lett.* **97**, 226401 (2006), [4] H. Bracht *et al. Phys. Rev. B* **75**, 035211 (2007)

HL 54.2 Fri 10:45 EW 202

Point defects in germanium - theory and experiment — •Sibylle Gemming, Clemens Wündisch, and Matthias Posselt — Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany.

The functionality of standard silicon-based semiconductor devices is achieved by careful point defect engineering, hence tremendous efforts have been made to arrive at a quantitative understanding of the underlying interactions. Germanium has distinct advantages over silicon, for instance the lower energy gap between occupied and empty electronic states and the resultant lower carrier injection barriers. However, germanium is less well studied than silicon. Thus, both theoretical and experimental investigations were carried out to study the interaction of point defects in germanium. Conductivity measurements of phosphorus-implanted germanium indicate that not all dopant atoms are electronically active. Therefore density-functional calculations were carried out to study the properties of Ge vacancies, substitutional phosphorus defects and their interaction. Stable defect clusters are obtained, and in the limit of high dopant concentration an electrically inactive form of the P dopant is predicted.

HL 54.3 Fri 11:00 EW 202

Red-shift in SiNW Raman spectra - influence from thermal properties — •Sevak Khachadorian, Harald Scheel, and Christian Thomsen — Institute für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

The Raman spectra of silicon nanowires are studied as a function of laser excitation power and temperature. With increasing temperature and laser excitation power we observe an amplification of the red-shift of the Raman frequency as well as of the broadening of the Raman peak. The Raman frequency varies linearly with the temperature. We observe a change of the slope in the frequency- excitation power diagram from a critical excitation power, which depends on the surrounding gas. From homogeneously heated experiments using a heating stage we find that the change of the slope in the frequency- excitation power diagram can be explained with inhomogeneous heating in the Raman volume generated by the Gaussian distribution of the intensity of the laser. With vacuum measurements we can rule out effects due to convection.

HL 54.4 Fri 11:15 EW 202

Atomistic simulation of amorphous germanium — •Alice-Agnes Gabriel and Matthias Posselt — Forschungszentrum Dresden-Rossendorf e. V.

Electrical doping of Ge is usually performed by ion implantation and subsequent annealing. In many cases ion bombardment leads to formation of an amorphous layer. During annealing the layer recrystallizes by solid-phase epitaxial regrowth. In order to investigate this process by classical molecular dynamics simulations, first of all amorphous Ge with realistic properties must be prepared. This is the subject of the present work. The atomistic simulations use the Stillinger-Weber interatomic potential with a parameter set that yields correct or reasonable structural, thermodynamic and defect properties of diamond-structure Ge. In the first simulation step liquid Ge is prepared. Then, the system is cooled down slowly to 300 K using the method of Luedtke and Landman which was applied to simulate amorphous silicon. Finally, an equilibration at 300 K and zero pressure is performed. The characterization of amorphous Ge obtained in this manner includes density and cohesive energy, radial distribution function and static structure factor, coordination number, bond-angle distribution, distribution of interatomic distances as well as melting temperature and heat of fusion. The simulation results show very good agreement with experimental data and are consistent with previous theoretical investigations.

HL 54.5 Fri 11:30 EW 202

Hydrogen passivation of low temperature polycrystalline silicon thin films for electronic applications — •Christian Jaeger, Tobias Antesberger, Michael Scholz, Matthias Bator, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

Polycrystalline silicon on low cost substrates is gaining importance for many applications of large area electronics. A promising method to obtain high quality polycrystalline Si films with a small thermal budget is the aluminum-induced layer exchange (ALILE) process. Here, an Al/oxide/amorphous Si layer stack is annealed at temperatures below 577 °C. This leads to an exchange of the position of the initial layers and the crystallization of the Si. Due to the high solid solubility of Al in Si, the resulting layers are highly p-doped. For most electronic applications such high carrier concentrations are not desirable. Therefore, the influence of hydrogen passivation on the electronic properties of thin poly-Si films prepared by ALILE has been investigated. We observe an increase of the resistivity after hydrogen passivation, which is the more pronounced, the thinner the samples. For the thinnest layers an increase of more than five orders of magnitude is observed. This is attributed to a combination of two effects - acceptor passivation by hydrogen and additional compensation of the free holes remaining after hydrogenation by interface states. The field effect in these passivated layers has been characterized in gated structures, both in bottom and top gate configuration. A significant field effect has been observed in H-passivated films with a thickness of 20 nm.

HL 54.6 Fri 11:45 EW 202

Proton irradiation of germanium isotope multilayer structures — •Sebastian Schneider[1], Hartmut Bracht[1], Martin Petersen[2], John Lundsgaard Hansen[2], and Arne Nylandsted Larsen[2] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

Irradiation of germanium (Ge) isotope heterostructures with 2.5 MeV protons have been performed at 550 deg C. The applied proton flux was varied between 1.0 and 1.5 microampere leading to various rates of Frenkel pair production. After rradiation, concentration profiles of the Ge-isotopes were recorded by means of secondary ion mass spectrometry. An inhomogeneous broadening of the isotope structure was observed that in addition to irradiation enhanced self-diffusion is affected by the formation of microscopic defects. Atomic force and scanning electron microscopy show that the microscopic defects are most probably resulting from an aggregation of vacancies formed during irradiation. Numerical analysis of Ge profiles not disturbed by microdefect formation indicates a significant contribution of self-interstitials to self-diffusion under irradiation.

HL 54.7 Fri 12:00 EW 202

Structural and electronic properties of ultra-thin polycrystalline Si layers on glass prepared by aluminum-induced layer exchange — •Tobias Antesberger, Christian Jäger, Michael Scholz, Chiara Cordioli, and Martin Stutzmann — Walter Schot-

tky Institut, Technische Universität München, Am Coloumbwall 3, 85748 Garching, Germany

Polycrystalline silicon thin films on low cost substrates are attractive for large area electronics and solar cell applications. A promising method to obtain large-grained high quality polycrystalline films by low-temperature crystallization of an amorphous precursor material is the aluminum-induced layer exchange (ALILE). In this approach, an Al/amorphous Si layer stack, separated by a thin oxide film, is annealed at temperatures below the Al-Si eutectic temperature of 850 K, leading to a complete exchange of the positions of the initial Al and Si layers and to the crystallization of the amorphous Si. We have studied the dynamics of the ALILE process as well as the structural and electronic properties of resulting ultra-thin polycrystalline Si layers (5 nm - 100 nm) prepared on silica substrates. Raman spectroscopy gives evidence of a good crystalline quality of the layers down to a thickness of 10 nm. Hall effect and conductivity measurements show a decreasing carrier density and an increasing mobility with increasing layer thickness. Due to the solubility of aluminum in silicon the resulting poly-Si layers are highly p-doped reaching carrier densities between 3x10^{18} cm^{-3} and 9x10^{19} cm^{-3} and hole mobilities up to 20 $cm^2/(Vs)$.

HL 54.8 Fri 12:15 EW 202

Oxidation and graphitization of 6H-SiC (0001) — Maxim Eremtchenko[1], Anita Neumann[1], Jens Uhlig[1], Rolf Öttking[1], Roland J. Koch[1], Katharina Kloeckner[1], Thomas Haensel[1], Syed Imad-Uddin Ahmed[1], and •Juergen A. Schaefer[1,2] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Department of Physics, Montana State University, P.O. Box 173840, Bozeman, MT 59717-3840, USA

The silicon rich 6H-SiC (0001) surface, its oxidation, graphitization and possible graphene layer formation has been investigated using high resolution electron energy loss spectroscopy in combination with X-ray induced photoelectron spectroscopy and low energy electron diffraction. Annealing up to 1000°C resulted in SiO_2 formation, while graphitization and finally the build up of graphitic clusters followed annealing up to 1170°C. Characteristic changes in surface cleanliness, stoichiometry (Si-rich to C-rich) and different surface structures induced drastically different depletion layers with different band bendings as a function of isochronal annealing temperatures. A key feature of this work is that the semimetallic character of graphite and/or graphene formation of intentionally low doped (2.5 x 10^{15} cm^{-3} n-type) SiC (0001) material could be precisely monitored by analyzing the continuous background of inelastically reflected electrons in HREELS-experiments. This result is very promising for future studies related to the identification of the presence and morphology of graphene layer formation on top of silicon carbide, and to its electronic as well as vibrational structure.

15 min. break

HL 54.9 Fri 12:45 EW 202

Grain boundary conduction in undoped laser-crystallized polycrystalline silicon-germanium thin films — •Lars-Peter Scheller[1], Moshe Weizman[1], Norbert H. Nickel[1], and B. Yan[2] — [1]Hahn-Meitner-Institut Berlin, Kekuléstr. 5, 12489 Berlin, Germany — [2]United Solar Ovonic Corporation, 1100 West Maple Road Troy, MI 48084, USA

Due to its enhanced optical absorption in the IR and visible spectral range polycrystalline silicon-germanium (poly-SiGe) is a promising absorber material for future thin film and tandem solar cells.
In this study the electrical transport properties of laser-crystallized poly-$Si_{1-x}Ge_x$ thin films ($0 \leq x \leq 1$) on quartz were investigated by temperature dependent Hall and conductivity measurements. All intentionally undoped samples showed p-type conduction that in some cases was accompanied by an astonishing high conductivity in the range of 0.1 to 10 $(\Omega cm)^{-1}$. Depending on the germanium content and the used crystallization procedure, three different transport mechanisms were identified: a) thermally activated transport with an activation energy of approximately 350 meV, b) Mott's variable range hopping and c) a nearly temperature independent metallic like transport. In addition, a subsequent remote hydrogen plasma treatment led to a pronounced decrease in the conductivity and a transition from metallic to activated transport. This surprising behavior is explained in terms of carrier transport in a defect band induced by Ge dangling bond defects at the grain boundaries.

HL 54.10 Fri 13:00 EW 202

Remote plasma process with independent control of physical and chemical etching of Si / Ge — •Helmut Lochner[1], Martin Amberger[2], Therese Chabert[2], Martin Sterkel[3], Walter Hansch[3], Markus Reinl[1], and Ignaz Eisele[1] — [1]Universität der Bundeswehr München, Institut für Physik — [2]PVA Tepla AG, Feldkirchen — [3]TU München

In the fabrication of electrical and mechanical devices there are several possibilities to structure the surface. An established and state of the art technology is dry etching with plasma-activated gases. There are differences in activation and the use of the plasma. The most important difference is either using a chemical effect or a physical effect for etching with advantages and disadvantages in each case. Although there are reactors combining both effects (e.g. reactive ion etching), you cannot separate them absolutely or control them decoupled.

In our experiments the advantages of the cold remote downstream plasma of the silicon star 12M (PVA Tepla AG, with a 2,45 GHz microwave radical generator) with pure chemical etching (fluorine radicals) were investigated. The process was supplemented with a physical etch component which is independent controllable. This concept was realized with an additional electrical field, called "BIAS". The "BIAS" creates and accelerates Ar ions and generates an ion beam towards the surface.

As a result, the etch rates on Si and Ge as well as the aspect ratio increase. Anisotropic etching of silicon can be achieved. Furthermore the etching of other materials like SiC becomes possible.

HL 54.11 Fri 13:15 EW 202

Electrical and optical properties of laser-crystallized polycrystalline silicon-germanium thin films — •Moshe Weizman[1], Lars-Peter Scheller[1], Norbert Nickel[1], and Baojie Yan[2] — [1]Hahn-Meitner-Institut Berlin, Kekuléstr. 5, 12489 Berlin, Germany — [2]United Solar Ovonic Corporation 1100 West Maple Road Troy, MI 48084, USA

The SiGe thin films investigated in this study were deposited on quartz by glow-discharge decomposition of a mixture of disilane, germane, and hydrogen and subsequently crystallized employing a XeCl excimer laser. Our investigations reveal that the grain boundaries in the poly-SiGe films critically influence the electrical and optical behavior of this material. Hall effect and electron spin resonance (ESR) measurements show evidence for the formation of a defect band on grain boundaries due to dangling bonds. This defect band appears preferably in Ge rich alloys with a critical dangling bond concentration of about $5 \cdot 10^{18}$ cm^{-3} and causes high metallic-like conductivities at low temperatures. Optical absorption measured with photothermal deflection spectroscopy (PDS) reveals a direct band gap characteristic that suggests the absorption occurs primarily at the grain boundaries. Sub-bandgap absorption indicates that the position of the neutrally charged dangling bond D^0 is about 150 meV above the valance band, which is probably the reason the Fermi level is pinned at the lower half of the bandgap and the layers exhibit p-type conductivity. We will discuss these surprising properties in terms of solar cell potential applications

HL 54.12 Fri 13:30 EW 202

Diffusion of Si and Ge in SiGe-isotope structures — •Rene Kube[1], Hartmut Bracht[1], John Lundsgaard Hansen[2], and Arne Nylandsted Larsen[2] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

The diffusion of Si and Ge in SiGe isotope heterostructures with Ge contents x = 0, 0.05, and 0.25 at.% were performed at temperatures between 870 and 1270 deg C. The concentration profiles of the stable Si- and Ge-isotopes were recorded by means of time-of-flight secondary ion mass spectrometry (Tof-SIMS). For all compositions, an Arrhenius type temperature dependence of diffusion was observed. The activation enthalpy of Si diffusion is equal to that of Ge diffusion. However, the preexponential factor of Si diffusion is lower. Our results are compared to radiotracer diffusion studies reported recently.

HL 54.13 Fri 13:45 EW 202

Dopant-induced states in two-dimensional semiconductors — •Philipp Ebert, Sebastian Landrock, and Knut Urban — Institut für Festkörperforschung, Forschunsgzentrum Jülich, 52425 Jülich

Intentionally inserted impurities, referred to as dopant atoms, are the lifeline of semiconductor devices. They provide free charge carriers

into the bands of the host crystal and thereby allow to tune almost all properties of semiconducting materials. These free carriers are generated by the introduction of localized states into the band gap. For suitable dopant atoms these states are close enough to the band edges, that either electrons from the valence band can thermally populate these states (acceptor type states) or electrons in these states can be thermally excited into the conduction band (donor type states). In order to address the origin of these states, we used scanning tunneling microscopy and spectroscopy to probe the local density of states above dopant atoms in a two-dimensional semiconducting $\sqrt{3}\times\sqrt{3}$ Ga overlayer on Si(111) substrates. We observe two dopant-induced states and additional changes in the density of states. Using a momentum dependent analysis we demonstrate that the presence of dopant atoms shifts parts of the local density of states. These results are discussed using existing models.

HL 54.14 Fri 14:00 EW 202

Phosphorus doping of Si nanocrystals — •Andre R. Stegner[1], Rui N. Pereira[1], E. Ulrich Stützel[1], Hartmut Wiggers[2], Martin S. Brandt[1], and Martin Stutzmann[1] — [1]Walter Schottky Inst., Technische Universität München, Garching — [2]Universität Duisburg-Essen, Inst. for Combustion and Gas Dynamics, Duisburg

Si nanocrystals (Si-ncs), in particular in the form of deposited or self-organized thin films are an interesting option for printed electronics and solar cells. However, the doping of individual Si-ncs, as well as its influence on the electronic properties of Si-ncs films is essentially unexplored. Here, we have used electron paramagnetic resonance (EPR) to study the P doping of Si-ncs grown by microwave-induced decomposition of silane and phosphine. EPR spectra of the as-grown Si-ncs show characteristic resonances from isolated as well as exchange-coupled P donors and an intense line originating from Si dangling bonds (Si-dbs) at the Si/SiO2 interface. While the P concentration determined with secondary ion mass spectroscopy is in good agreement with the doping level calculated from the phosphine concentration during synthesis, a quantitative analysis of the EPR data reveals that only a small fraction of the donors contributes to the characteristic EPR signal. This discrepancy increases strongly for Si-ncs smaller than 15 nm and is discussed taking into account effects like self purification and charge compensation by Si-dbs. Using electrically detected magnetic resonance to study the spin-dependent transport in thin films of Si-ncs, we show that P donor states in the core of the Si-ncs and Si-dbs at the nanocrystal surface are actively involved in the current transport.

HL 54.15 Fri 14:15 EW 202

Diffusion and defect reactions between donors, carbon and vacancies in germanium — •Hartmut Bracht[1], Sergej Brotzmann[1], John Lundsgaard Hansen[2], and Arne Nylandsted Larsen[2] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Department of Physics and Astronomy, University of Aarhus, Denmark

The diffusion of self-atoms and n-type dopants such as phosphorus (P), arsenic (As), and antimony (Sb) was studied by means of isotopically controlled germanium multilayer structures doped with carbon. The diffusion profiles reveal an aggregation of the dopants within the carbon-doped layers and a retarded penetration depth compared to dopant diffusion in high purity natural Ge. Dopant aggregation and diffusion retardation is strongest for Sb and similar for P and As. In addition, the shape of the dopant profiles changes for high dopant concentrations. Accurate modeling of the simultaneous self- and dopant diffusion is achieved on the basis of the vacancy mechanism and additional reactions that take into account the formation of neutral carbon-vacancy-dopant and neutral dopant-vacancy complexes. The stability of these complexes is compared to recent theoretical calculations. The overall consistency between the experimental and theoretical results support the stabilization of donor-vacancy complexes in Ge by the presence of carbon and the dopant deactivation via the formation of dopant-vacancy complexes.

HL 54.16 Fri 14:30 EW 202

MBE-growth and characterization of highly P doped delta layers in silicon — •Ulrich Abelein, Peter Iskra, Martin Schlosser, Torsten Sulima, and Ignaz Eisele — Universtität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

The controlled and reproducible growth of highly doped and ultra thin delta layers in silicon by MBE is an important task for the study of a wide range of phenomena in semiconductor physics (like resonant tunneling) as well as for the development of novel devices (like the TFET or the vertical I-MOS).

While the fabrication of boron doped delta layers with excellent electrical properties is quite well understood, the preparation of phosphorus doped delta layers is more difficult. High phosphorus doping leads to the formation of phosphorus clusters which cause crystal defects and degenerate electrical properties. In this work 3 nm thick delta layers with doping levels $> 10^{20}$ cm^{-3} were grown by MBE and characterized using secondary ion mass spectroscopy (SIMS). Furthermore such delta layers were used to fabricate triangular barrier diodes (TBD, i. e. p^+-i-n^+-δ-i-p^+ layer stacks). The electrical characteristics of these test devices show a very good barrier formation by the delta layers which indicates good crystal quality.

HL 54.17 Fri 14:45 EW 202

Einfluss der Dotierung auf die elastischen Eigenschaften von Silizium — •Nicole Santen und Reiner Vianden — Helmholtz - Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Für die Herstellung von Hochleistungshalbleiterbauelementen wird heutzutage sog. *strained silicon*, also gedehntes Silizium, verwendet. Dadurch ist es möglich die Ladungsträgerbeweglichkeit und damit die Schaltgeschwindigkeiten von Transistoren zu erhöhen und eine Verbesserung der Gesamtleistung zu erzielen.

Die Methode der gestörten γ-γ-Winkelkorrelation (PAC) ist sehr gut für die Untersuchung solcher lokaler Verspannungen in Silizium geeignet, da sie mikroskopische Beobachtungen der unmittelbaren Umgebung eines Sondenkerns ermöglicht. Auf diese Art können zum einen extern angelegte Zug- und Druckspannungen untersucht werden, aber auch Gitterverzerrungen, wie sie in implantierten Bereichen auftreten.

Mit der PAC-Sonde ^{111}In wird der Einfluss von Dotierungsatomen auf die elastischen Eigenschaften von Silizium untersucht. Frühere Messungen weisen darauf hin, dass das Siliziumgitter abhängig von der Art der Dotierungsatome unterschiedlich auf eine mechanische Verspannung reagiert. Neuere Messungen zeigen, dass man durch Implantation von Donatoren und Akzeptoren die elastischen Eigenschaften unterschiedlich beeinflussen kann. Dies wird anhand von Phosphor- und Bor-dotiertem Silizium verdeutlicht.