HL 39: Group IV (other than C): Si/Ge/SiC

Time: Thursday 11:00–13:00 Location: EW 015

HL 39.1 Thu 11:00 EW 015

investigation of 3C-SiC/SiO2 interfacial point defects from first principles calculations and electron paramagnetic resonance measurements — •Taufik Adi Nugraha[1,2], Martin Rohrmüller[2], Uwe Gerstmann[2], Siegmund Greulich-Weber[3], Jean-Louis Cantin[4], Jurgen von Bardeleben[4], Wolfgang Gero Schmidt[2], and Stefan Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung — [2]University of Paderborn — [3]Solar Weaver GmbH — [4]University Pierre and Marie Curie

SiC is widely used in high-power, high-frequency electronic devices. It has also been used as a building block in hybrid nanocomposites for photovoltaics. Analogous to Si, SiC features SiO2 as native oxide that can be used for passivation and insulating layers. However, a significant number of defect states are reported to form at SiC/SiO2 interfaces, limiting mobility and increasing recombination of free charge carriers. Combining ab initio g-tensor and hyperfine interactions calculations with electron paramagnetic resonance (EPR) measurements, we show that carbon antisite dangling bond (Csi-db) defects explain the measured EPR signatures. Csi-db is found to be strongly stabilized at the interface, because carbon changes its hybridization from sp3 in the SiC- bulk to sp2 at the interface, creating a dangling bond inside a porous region of the SiO2 passivating layer. The calculated energy level of a neutral Csi-db coincides with the barrier height of the interface states from internal photoemission (IPE) of SiC/SiO2 interfaces, indicating a contribution of Csi-db to the measured interface states.

HL 39.2 Thu 11:15 EW 015

Towards room-temperature extended infrared Si-based photoresponse: A case study of Te-hyperdoped Si — •Mao Wang[1,2], Yonder Berencén[1], Slawomir Prucnal[1], Eric García-Hemme[3], René Hübner[1], Ye Yuan[1,2], Chi Xu[1,2], Lars Rebohle[1], Roman Böttger[1], René Heller[1], Harald Schneider[1], Wolfgang Skorupa[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany — [3]Univ. Complutense de Madrid, Departamento de Física Aplicada III (Electricidad y Electrónica), 28040 Madrid, Spain

Presently,room-temperature broadband Si-based photodetectors are required for Si photonic systems.Here,we demonstrate room-temperature sub-band gap photoresponse of photodiodes based on Si hyperdoped with Te.The epitaxially recrystallized Te-hyperdoped Si layers are developed by ion implantation combined with pulsed laser melting and incorporate Te concentrations beyond the solid solubility limit.An insulator-to-metal transition driven by increasing Te concentration accompanied with a band gap renormalization is observed.The optical absorptance is found to increase monotonically with increasing Te concentration and extends well into the mid- and far- infrared regions.This work contributes to establish room temperature Si-based broadband infrared photonic system.

HL 39.3 Thu 11:30 EW 015

Crystal phase effects in group IV nanowire polytypes and their homojunctions — •Michele Amato — Laboratoire de Physique des Solides (LPS) Centre de Nanosciences et de Nanotechnologies (C2N) Université Paris-Sud, Orsay (France)

Recent experimental investigations have confirmed the possibility to synthesize and exploit polytypism in group IV nanowires. Indeed, while the crystal structure of Si and Ge nanowires (NWs) at standard conditions usually takes a well-defined cubic-diamond phase (as for their bulk counterparts), in the last few years several experimental observations of NWs exhibiting other phases - i.e. the hexagonal-diamond one - have been reported [1-2]. Driven by this promising evidence, here I will discuss recent first-principles calculations of the electronic and optical properties of hexagonal-diamond and cubic-diamond Si and Ge NWs as well as their homojunctions [3-4]. I will outline how a change in the crystal phase can strongly modify the electronic structure and optical response of the NW inducing novel and fascinating properties. Furthermore, I will show that, in the case of homojunctions, playing on crystal phase, size and length of the junction is an efficient tool to modulate band offsets and electron-hole separations.

References

[1] S. Assali et al., Nano Lett. 15, 8062-8069 (2015)
[2] J. Tang et al., Nanoscale, 9, 8113-8118 (2017)
[3] M. Amato et al., Nano Lett. 16, 5694-5700 (2016)
[4] T. Kaewmaraya et al., J. Phys. Chem. C 121, 5820-5828 (2017)

HL 39.4 Thu 11:45 EW 015

Shell-Thickness Controlled Semiconductor-Metal Transition in Si-SiC Core-Shell Nanowires — •Michele Amato — Université Paris-Sud, Orsay, France

Today Si nanowires (NWs) represent a viable solution to realize high-performance sensors due their potential for fabrication into high density nanoscale devices [1]. The large surface-to-volume ratio and the possibility to tune their properties at growth time controlling the composition, crystal orientation, and diameter make Si NWs bound to outperform any other conventional alternative in a large class of sensing environments [1]. On the other hand, because of its excellent chemical and mechanical stability, high hardness and low density it is widespread belief that SiC is a much better biocompatible material than Si. The combination of Si and SiC in a nanostructure, as shown by recent experiments [2], could lead therefore to a material with the smart properties of Si and the biocompatibility of carbon-based systems. We study Si-SiC core-shell NWs by means of electronic structure first-principles calculations [3]. We show that the strain induced by the growth of a lattice mismatched SiC shell can drive a semiconductor-metal transition. Core-shell nanowires with thicker cores, however, remain semiconducting even when four SiC monolayers are grown, paving the way to versatile, biocompatible nanowire-based sensors.

[1] M. Amato and R. Rurali, Prog. Surf. Sci. 91, 1-28 (2016) [2] L. Latu-Romain and M. Ollivier, J. Phys. D, 47, 203001 (2014) [3] M. Amato and R. Rurali, Nano Lett. 15, 3425 (2015)

HL 39.5 Thu 12:00 EW 015

Sub-Bandgap Photoluminescence Study on Implantation-Induced Color Centers in 4H-SiC — •Maximilian Rühl, Christian Ott, Michael Krieger, and Heiko B. Weber — Department of Physics, Chair of Applied Physics, FAU Erlangen-Nürnberg, Germany

Silicon carbide (SiC) is a promising host material for novel quantum technology based on single photon sources such as color centers in crystals [1]. In this study, we report on low temperature photoluminescence (PL) spectra related to color centers created by proton implantation and subsequent annealing. Particularly, we monitor the dependence of PL spectra on the implantation dose and the annealing temperature in a wide parameter range. Among the well known defect signatures related to the silicon vacancy (V_{Si}) defect and the carbon vacancy antisite (C_{Si}-V_C) defect we observe several omnipresent and highly temperature stable spectral lines (TS lines) three of which (at 768 nm, 811 nm and 813 nm) show strongly correlated PL intensities through all measurement parameters. This suggests a common underlying microscopic defect. Further, the intensities of the TS lines turn out to be clearly dependent on the initial implantation dose where the PL lines do not increase until an annealing temperature of 1200°C. At this temperature the initially created V_{Si} defects are basically annealed, hence the defect responsible for the TS signature could be a transformation product of the afore-mentioned.

[1] S. Castelletto *et. al.* nature materials 13, 151-156 (2013)

HL 39.6 Thu 12:15 EW 015

electronic and optical properties of hexagonal germanium: influence of echange and correlation — •valerio armuzza, jürgen furthmüller, claudia rödl, friedhelm bechstedt, and silvana botti — Institut für Festkörpertheorie und Optik der Friedrich-Schiller-Universität, Jena, Jena, Germany

Using ab initio density functional calculations, we study the effect of several Exchange and Correlation (XC) potentials on geometry, electronic and optical properties of Cubic (C) and Lonsdaleite (L) Germanium (Ge), including spin-orbit interaction and d-electrons. Given the importance of Ge in semiconductor technology, this work is directed to the best approach comparing with the well-known experimental results for C-Ge. It is applied on the L-Ge polytype. We initially obtain the

lattice parameters, cohesive energies and bulk moduli with the LDA, PBE, PBEsol and AM05 potentials, while, subsequently the energy band gaps, band structures, optical transitions and radiative lifetimes are calculated with the PBEsol, a *hybrid* XC-funcional (HSE06) and a *meta*-GGA functional (MBJLDA). The atomic geometry for PBEsol and AM05 are consistent with experimental results. Band gaps are slightly overestimated (underestimated) for HSE06 (MBJLDA) in C-Ge, while we have the opposite situation in L-Ge. The small lonsdaleite gap and the symmetry of the lowest conduction bands are explained in terms of folding of the diamond-structure bands.

HL 39.7 Thu 12:30 EW 015

Phase separation in metastable $Ge_{1-x}Sn_x$ epilayers induced by free running Sn precipitates — •Heiko Groiss[1,2,3], Martin Glaser[2], Magdalena Schatzl[2], Moritz Brehm[2], Dagmar Gerthsen[3], and Friedrich Schäffler[2] — [1]Center of Surface and Nanoanalytics, Johannes Kepler University Linz, Austria — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria — [3]Laboratory for Electron Microscopy, Karlsruhe Institute of Technology, Germany

Recently, optical gain was demonstrated in $Ge_{1-x}Sn_x$ alloys [1], which are the only known group-IV materials that assume a direct band gap. However, Ge and Sn are immiscible over 98% of the composition range, which renders these epilayers inherently metastable. We investigated the temperature stability of pseudomorphic $Ge_{0.9}Sn_{0.1}$ films grown by MBE [2]. We observed that decomposition of the epilayers sets in above 230°C, the melting point of Sn. Videos taken during annealing in a scanning electron microscope reveal the crucial role of liquid Sn precipitates. Driven by a gradient of the chemical potential, the Sn droplets move on the surface and behave like microscopic liquid-phase epitaxy reactors: The strained and metastable GeSn film on the one side acts as a feeding medium for the supersaturation of the Sn melt with Ge. From this Sn melt Ge precipitates epitaxially in a trail region, where it develops low energy facets. Overall, the free-running Sn droplets make phase separation of metastable GeSn layers particularly efficient at rather low temperatures. [1] S. Wirths *et al.*, Nat. Photonics **9**, 88-92 (2015). [2] H. Groiss *et al.*, Scientific Reports **7**, 16114 (2017).

HL 39.8 Thu 12:45 EW 015

High-resolution patterning of germanium for nanoelectronics applications — Anushka S. Gangnaik[1], Muhammad Bilal Khan[2], Shima J. Ghamsari[2], Lars Rebohle[2], Artur Erbe[2], Justin D. Holmes[1], and •Yordan M. Georgiev[2] — [1]Materials Chemistry and Analysis Group, School of Chemistry and Tyndall National Institute, University College Cork, Cork, Ireland and AMBER@CRANN, Trinity College Dublin, Dublin 2, Ireland — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstrasse 400, 01328 Dresden, Germany

Ge is among the most attractive alternative channel materials for the next-generation nanoelectronics. However, Ge patterning with electron beam lithography (EBL) using the negative resist HSQ is challenging. The complex native oxide GeOx is soluble in the HSQ aqueous developers. As a result, lift-off of sub-20 nm features written by EBL occurs during development. In the presentation, it will be shown that this issue can be solved by: (i) removal of GeOx and passivation of Ge surface prior to HSQ deposition or (ii) application of a buffer layer between GeOx and HSQ. Arrays of sub-20 nm HSQ lines were successfully fabricated on Ge with both approaches. Moreover, a significantly simplified process for removal of GeOx and passivation of Ge surface will also be presented, which allows patterning of 6-7 nm Ge NWs, the smallest Ge nanostructures reported to date.

Finally, different applications of the above mentioned patterning processes will be discussed.