HL 74: Group IV: Si/Ge/SiC

Time: Thursday 12:00–13:15 Location: POT 06

HL 74.1 Thu 12:00 POT 06

The silicon path to a new kilogram: Impact of the isotopic composition of Si determined by high resolution mass spectrometry — •Axel Pramann and Olaf Rienitz — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

The planned re-definition of the SI unit kilogram will be performed via the Planck constant h and in a complementary approach via the Avogadro constant N_A applying the X-ray-crystal-density XRCD method (Avogadro-project) by counting the silicon atoms in single-crystalline Si spheres[1]. One key experiment is the mass spectrometric determination of the molar mass M of Si with lowest uncertainty by developing new analytical techniques (isotope ratio calibration) and modifying e.g. isotope dilution mass spectrometry (IDMS) in combination with a high resolution multicollector-ICP-mass spectrometer (HR-MC-ICP-MS) [2]. This resulted in u_rel(M) < 5 x 10-9 routinely, when applied to silicon material enriched in 28Si with x(28Si) > 0.9999 mol/mol. New Si crystals even higher enriched in 28Si recently produced in Russia exhibit a strong reduction of u(M). Already u_rel(M) < 1 x 10-9 can be obtained when using crystals with x(28Si) > 0.999 99 mol/mol. An estimation of the correlation between enrichment and decrease of uncertainty is given, stimulated by an uncertainty reduction of M by approximately three orders of magnitude in ten years [3].

[1] Y. Azuma et al., Metrologia, 52, 360 (2015). [2] O. Rienitz, A. Pramann, D. Schiel, Int. J. Mass Spectrom., 289, 47 (2010). [3] K. Fujii et al. Metrologia, 53, A19 (2016).

HL 74.2 Thu 12:15 POT 06

Modulation Doping of Si using Al-induced Acceptor States in SiO2 — Dirk König[1], •Daniel Hiller[2], Sebastian Gutsch[2], Margit Zacharias[2], and Sean Smith[1] — [1]University of New South Wales (UNSW), Sydney, Australia — [2]Laboratory for Nanotechnology, IMTEK, University of Freiburg, Germany

Silicon nanovolumes suffer from effects that impede conventional doping due to fundamental physical principles such as out-diffusion, statistics of small numbers, quantum- or dielectric confinement. Efficient and reliable control over the majority charge carriers by impurity doping is infeasible for ultra-small Si crystals [1].

In this work, we demonstrate a heterostructure modulation doping method for Si, similar to the concept of modulation doping originally invented for III-V semiconductors [2]. Our approach utilizes a specific acceptor state of Al-atoms in SiO2, which is located 0.5 eV below the Si valence band, to generate holes as majority carriers in adjacent Si [3]. The relocation of the impurity dopants from Si to SiO2 circumvents all nanoscale doping problems. We present successful Si modulation doping from the theoretical background (density functional theory simulations, DFT) to experimental evidence by capacitance-voltage (C-V), Hall-measurements and deep level transient spectroscopy (DLTS). In addition, we demonstrate how modulation doping of bulk-Si enables passivating hole selective tunnelling contacts as required for high-efficiency photovoltaics [3].

[1] Sci. Rep. 5, 09702 (2015) [2] Appl. Phys. Lett. 33, 665 (1978) [3] D. König & D. Hiller et al., Sci. Rep., under review (2016)

HL 74.3 Thu 12:30 POT 06

Investigation of 3C-SiC/SiO2 interfacial point defects from ab initio g-tensor calculations and electron paramagnetic resonance measurements — •T. A. Nugraha[1,2], M. Rohrmüller[2], U. Gerstmann[2], S. Greulich-Weber[3], A. Stellhorn[2], J. L. Cantin[4], J. Von Bardeleben[4], W. G. Schmidt[2], and S. Wippermann[1] — [1]Max-Planck-Institut für Eisenforschung — [2]University of Paderborn — [3]Solar Weaver GmbH — [4]Pierre and Marie Curie University

SiC is widely used in high-power, high-frequency electronic devices. Recently, it has also been used in nanocomposites as light absorbers in solar energy conversion devices. 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. We investigated the growth of oxide on different 3C-SiC surfaces from first principles. Carbon antisite Csi defects are found to be strongly stabilized in particular 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. Combining ab initio g-tensor calculations and electron paramagnetic resonance (EPR) measurements, we show that Csi defects explain the measured EPR signatures, while the hyperfine structure allows to obtain local structural information of the oxide layer. Financial support from BMBF NanoMatFutur grant 13N12972 and DFG priority program SPP-1601 is gratefully acknowledged.

HL 74.4 Thu 12:45 POT 06

Direct band gap and strain-related properties of germanium under high uniaxial stress — •Kevin Guilloy[1], Alban Gassenq[1], Nicolas Pauc[1], S. Tardif[1], F. Rieutord[1], Y.M. Niquet[1], J.M. Escalante[1], I. Duchemin[1], L. Milord[2], G. Osvaldo Dias[2], D. Rouchon[2], J. Widiez[2], J.M. Hartmann[2], J. Aubin[2], A. Chelnokov[2], R. Geiger[3], T. Zabel[3], E. Marin[3], H. Sigg[3], J. Faist[4], V. Reboud[2], and Vincent Calvo[1] — [1]Université Grenoble Alpes, CEA-INAC, Grenoble, France — [2]Université Grenoble Alpes, CEA-LETI Minatec, Grenoble, France — [3]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, Villigen, Switzerland — [4]Institute for Quantum Electronic, ETH Zurich, Switzerland

The induction of high tensile strain is predicted to make germanium a direct band gap semiconductor. We present here an experimental study of the dependence of such a tensile stress on the direct optical transitions and the Raman strain-induced shift.

Using germanium-on-insulator (GeOI) substrates, we fabricated micro-membranes amplifying the residual stress of the germanium layer. Laue X-ray diffraction measurements at the BM32 beamline (ESRF) showed the strain reaches 4.9 %. We studied the relationship between the strain measured by XRD and the Raman shift and observed a unexpected nonlinear behaviour.

We finally performed electro-absorption spectroscopy on micro-bridges to determine the energy of its optical transitions, showing that the relation between strain and the energy of these transitions differs significantly from previous models.

HL 74.5 Thu 13:00 POT 06

Defect-induced magnetism in SiC probed by nuclear magnetic resonance — •Zhitao Zhang[1,2], Daryna Dmytriieva[2,3], Sebastian Molatta[2,3], J. Wosnitza[2,3], Yutian Wang[1], Manfred Helm[1,3], Shengqiang Zhou[1], and Hannes Kühne[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [3]TU Dresden, D-01062 Dresden, Germany

We give evidence for intrinsic, defect-induced bulk paramagnetism in SiC by means of ^{13}C and ^{29}Si nuclear magnetic resonance (NMR) spectroscopy. The temperature dependence of the internal dipole-field distribution, probed by the spin part of the NMR Knight shift and the spectral linewidth, follows a Curie law and scales very well with the macroscopic DC susceptibility. In order to quantitatively analyze the NMR spectra, a microscopic model based on dipole-dipole interactions was developed. The very good agreement between these simulations and the NMR data establishes a direct relation between the frequency distribution of the spectral intensity and the corresponding real-space volumes of nuclear spins. The presented approach by NMR can be applied to a variety of similar materials and, thus, opens a new avenue for the microscopic exploration and exploitation of diluted bulk magnetism in semiconductors.