HL 25 Si / Ge

Zeit: Samstag 10:45–12:45 Raum: TU P-N226

HL 25.1 Sa 10:45 TU P-N226

Grazing-Incidence Diffraction Strain Analysis of a Laterally patterned Si wafer treated by Focused Ge and Au Ion Beam Implantation — •J. Grenzer[1], L. Bischoff[1], and U. Pietsch[2] — [1]Forschungszentrum Rossendorf e.V., Institute of Ion Beam Physics and Materials Research,P.O.Box 51 01 19, D-01314 Dresden, Germany — [2]University of Potsdam, Institute of Physics, Am Neuen Palais 10, 14469 Potsdam, Germany

Strain analysis of a laterally patterned Si-wafer was carried out utilizing X-ray grazing-incidence diffraction performed at the ID10B at the ESRF. The lateral patterning was done by focused ion beam implantation using a AuGeSi alloy liquid metal ion source. Samples were prepared by either a 35 keV Au^+ ion beam (dose: $0.3, 2 \cdot 10^{14} cm^{-2}$) or by a 70 keV Ge^{++} ion beam (dose: $8 \cdot 10^{14} cm^{-2}$). It was shown that a periodical defect structure consisting of both implanted and not implanted stripes is created due to ion beam implantation. The induced strain distribution induced, however, shows no periodicity. This can be only explained by an overlap of the strain fields created in each implanted stripe.

We found a maximum strain for the Au implanted samples in a depth of about 20 nm ($\Delta a/a = -1, -3 \cdot 10^{-4}$ for the Au samples); for the Ge sample in a depth of $\approx 100nm$ ($\Delta a/a = -1.2 \cdot 10^{-4}$). At depths $500nm$ below the sample surface the strain of the Ge sample becomes smaller than the detection limit ($\Delta a/a < 2 \cdot 10^{-5}$). Using this technique we were able to create a buried Ge layer with a thickness of about 200 nm and an averaged Ge content of about 1%.

HL 25.2 Sa 11:00 TU P-N226

Doppelresonantes Raman Spektrum in Germanium — •M. Mohr, M. Machón, J. Maultzsch und C. Thomsen — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin

Das Raman Spektrum von Germanium zeigt eine schwache Mode unterhalb der optischen Phononen, deren Frequenz von der Energie der Anregung abhängt[1]. Diese Abhängigkeit ist je nach Orientierung der Probe verschieden. Wir haben diese Mode in Hinsicht auf Doppelresonanz[2] untersucht. Nach der resonanten Absorption von Licht wird das Elektron in einen realen Zustand gestreut, was zu einer zweifachen Verstärkung des Ramansignals führt. Die im Prozess beteiligten Phononen stammen nicht aus dem Γ-Punkt, daher können über die Phononendispersion Rückschlüsse gezogen werden. Wir untersuchen die Streuprozesse entlang Achsen hoher Symmetrie, diskutieren den Einfluss der Auswahlregeln für Elektron-Phonon-Streuung und vergleichen die Vorhersagen mit experimentellen Daten.
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[1] D.J. Mowbray et al., Proc. 20th ICPS (World Scientific, 1990), 2017
[2] C. Thomsen und S. Reich, Phys. Rev. Lett. **85**, 5214 (2000)

HL 25.3 Sa 11:15 TU P-N226

Vacancy complexes with oversized impurities in Si and Ge — •K. Schroeder, H. Höhler, N. Atodiresei, R. Zeller, and P. H. Dederichs — Institut für Festkörperforschung, FZJ, 52425 Jülich

We examine the electronic and geometrical structure of impurity-vacancy complexes in Si and Ge. Within the framework of density-functional theory we use two complementary *ab initio* methods, the pseudopotential-PW method and the all-electron KKR method, to investigate the structure of vacancy complexes with 11 different *sp*-impurities. For Sn in Si, we confirm the split configuration (Sn on the bond center and two half vacancies on neighboring sites), and obtain good agreement with EPR data of Watkins[1]. We find that all impurities of the 5*sp* and 6*sp* series in Si and Ge prefer the split-vacancy configuration, with an energy gain of 0.5 to 1 eV compared to the substitutional complex. On the other hand, impurities of the 3*sp* and 4*sp* series form (slightly distorted) substitutional complexes. An exception from this rule is Al, which forms a split complex in Si and a strongly distorted substitutional complex in Ge. We find a strong correlation of these data with the size of the isolated impurities, defined via the lattice relaxations of the nearest neighbors.

[1] G. D. Watkins, Phys. Rev. B **12**, 4383 (1975)

HL 25.4 Sa 11:30 TU P-N226

Electronic and optical properties of capped Si and Ge nanocrystallites — •Luis Ramos, Jürgen Furthmüller, and Friedhelm Bechstedt — FSU Jena - IFTO, Max-Wien-Platz 1, D-07743 Jena, Germany

Quantum confinement (QC) in Si and Ge nanocrystallites (NC's) gives rise to new material properties interesting to applications such as data storage devices, photodetectors, and optoelectronics. The lattice mismatch of Si and Ge and the fact that $Si_{1-x}Ge_x$ is a highly miscible alloy for all concentrations x could prevent very sharp Si/Ge interfaces. However, a considerable progress in controlling the growth of Si/Ge heterostructures has been achieved and novel structures with embedded NC's can be synthetised.

In this work we present ab-initio pseudopotential plane-wave calculations for Si(Ge)-capped Ge(Si) free-standing NC's. We study their structural and electronic properties, optical absorption spectra, Stokes shifts, radiative lifetimes, and the space localization of the HOMO and LUMO. We verify that Si-(Ge-)capped Ge(Si) NC's have significant differences in their structures and the type-II character of a Si/Ge heterojunction. In certain cases the absorption spectra shows a compensation effect related to composition and QC effects. The results are compared to those of Si NC's capped with oxide shells.

HL 25.5 Sa 11:45 TU P-N226

Ripple structure of ion beam induced Si wafer — •Ullrich Pietsch[1], J. Grenzer[1], S. Hazra[2], T.K. Chini[2], and M.K. Sanyal[2] — [1]University of Potsdam, Institute of Physics, 14415 Potsdam, Germany — [2]Surface Physics Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700 064, India

Ion beam induced ripple formation in Si wafers was studied by atomic force microscopy (AFM) and non-destructive depth-resolved x-ray grazing incidence diffraction (GID). The formation of ripple structure at high doses ($\tilde{7}$x10 17 ions/cm2), starting from initiation at low doses ($\tilde{1}$x10 17 ions/cm2) of ion beam is evident from AFM, while that in the buried crystalline region below a partially crystalline top layer is evident from GID study. The GID technique reveals that these periodically modulated wave-like buried crystalline features become highly regular and strongly correlated as one increases the Ar ion beam energy from 60 keV to 100 keV. The vertical density profile obtained from the analysis of Vineyard profile shows that the density in the upper top part of ripples is decreased to about 15% of the crystalline density. The partially crystalline top layer at low dose, transforms to a completely amorphous layer for high doses and the top morphology was found to be conformal with the underlying crystalline ripple. On the other hand, the amorphous part of the damaged top layer is textured and scales with the ion dose. S. Hazra, T.K. Chini, M.K. Sanyal, J. Grenzer and U. Pietsch, Phys.Rev.B70 121307(R) 2004

HL 25.6 Sa 12:00 TU P-N226

X-ray Raman scattering at the Si L-edge of Si and amorphous SiO — •M. Volmer[1], C. Sternemann[1], J.A. Soininen[2], A. Hohl[3], G. Venko[4], S. Streit[1], and M. Tolan[1] — [1]Institut für Physik, Universität Dortmund, Deutschland — [2]Div. X-ray Physics, Dept. Physical Sciences, University of Helsinki, Finland — [3]Institute of Materials Science, Darmstadt University of Technology, Germany — [4]ESRF, Grenoble, France

We present measurements of the Si L-edge of polycrystalline Si and amorphous SiO using the x-ray Raman scattering technique (XRS). The momentum transfer dependence of XRS gives acces to additional monopole excitation channels for the high momentum transfer regime, where the dipole approximation is no longer valid. The Si L-edge spectra show clear momentum transfer dependence with respect to their total shape and will be compared to calculations using a Bethe-Salpeter equation-based approach including core-hole and lifetime effects. The Si L-edge of amorphous SiO exhibits distinct fine structure along with pronounced momentum-transfer dependence. These spectra will be discussed in terms of the interface-clusters mixture model for the structure of amorphous SiO on the basis of a disproportionation of SiO into Si and SiO_2.

HL 25.7 Sa 12:15 TU P-N226

Phosphorous donor wave function in strained silicon layers
— •Hans Huebl[1], André Stegner[1], Martin S. Brandt[1], and Günther Vogg[2] — [1]Walter Schottky Institut, Technische Universität München, München, Germany — [2]Fraunhofer Institut - Zuverlässigkeit und Microintegration, München, Germany

The wave function of shallow donors such as phosphorous in silicon can be determined very accurately by electron spin resonance. In particular in the context of quantum computing, the manipulation of the donor wave function currently receives considerable attention. Here, we report on the influence of strain on the hyperfine interaction in P-doped Si. In contrast to previous experiments, where the effects of external strain on bulk Si:P were investigated, we use fully strained thin Si:P layers on virtual SiGe substrates grown by CVD where high Ge contents of up to 30% in the substrate allow much higher strains to be investigated. For detection of the spin resonance in these thin epilayers, electrically detected magnetic resonance is used. Si:P on relaxed $Si_{0.84}Ge_{0.16}$ has a hyperfine interaction of 25 G, which is reduced by 40% from the unstrained case, in excellent agreement with the extrapolation of the data obatined on bulk Si:P.

HL 25.8 Sa 12:30 TU P-N226

Ferromagnetic Mn–doped Ge
— •Thomas Vallaitis, Mario Gjukic, Christian Jäger, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

Heavily manganese–doped germanium with a reported Curie temperature T_C of up to 116 K [Park *et al.*, Science **295** (2002), 651] is of interest as a potential material for spintronic applications. Samples have been grown on Ge(100) substrates by MBE with manganese concentrations ranging from 0.02 at.% up to 52 at.%, as determined by elastic recoil detection analysis and EDX. The substrate temperature was approx. 225 °C. Raman scattering and UV/VIS reflection measurements indicate a good crystalline quality of the epitaxial films up to a Mn concentration of 10 at.%, where the Ge TO Raman peak shows a FWHM of 5.4 cm^{-1}. Raman modes attributed to Mn–Mn vibrations as well as a low concentration of holes in Hall effect measurements indicate that clusters or intermetallic compounds are formed. SQUID magnetization measurements for samples with a Mn concentration of $3-20$ at.% clearly show the presence of several magnetic phases: (i) the ferromagnetic Mn_5Ge_3 with $T_C = 285$ K and (ii) a low–temperature phase with a remanence that disappears at 30 K.