

HL 63: Group IV elements and compounds

Time: Thursday 9:30–11:30

Location: EW 015

HL 63.1 Thu 9:30 EW 015

Selective formation of nano-GeSn(Si) structures on nano-patterned-Si(001) — ●V. SCHLYKOW^{1,2}, N. TAOKA¹, M. ZÖLLNER¹, O. SKIBITZKI¹, Y. YAMAMOTO¹, G. NIU¹, P. ZAUMSEIL¹, G. CAPELLINI^{1,3}, and T. SCHROEDER^{1,4} — ¹IHP, 15236 Frankfurt (Oder), Germany — ²University Leipzig, Germany — ³Università degli Studi Roma Tre, Italy — ⁴BTU Cottbus, Germany

The GeSn(Si) alloy is one of the key materials to link electrical and optical devices. Sn introduction makes it possible to change the energy band structure, making group IV materials suitable for optical device applications. However, crystalline defects due to lattice mismatch between GeSn(Si) and Si are a crucial problem hindering the realizing of optical devices. Recently, we have established an advanced heteroepitaxy approach to achieve fully coherent, dislocation-free Ge/SiGe/Si structures formed on nano-patterned Si(NP-Si) substrates. In this study we form nano-GeSn(Si) structures at low temperature with hydrogen plasma(HP). To confirm the possibility of selective MBE growth of Ge and Sn on Si or SiO₂ surface, deposition rates of Ge and Sn on Si or SiO₂ surfaces were investigated. RHEED and XPS clarified that the Ge deposition rate on the Si surface in HP at 300 °C is much higher than that on the SiO₂ surface. A Sn signal in XPS could not be detected after Sn deposition on the SiO₂ surface in HP. These results indicate that a window for (nearly) selective MBE growth can be achieved in HP to form nano-GeSn(Si) crystals on NP-Si. Post treatments for selective deposition of the alloy are part of ongoing investigations.

HL 63.2 Thu 9:45 EW 015

Valence band offset in heterojunctions between crystalline silicon and amorphous silicon (sub)oxides — ●MARTIN LIEBHABER, MATHIAS MEWS, TIM SCHULZE, LARS KORTE, and KLAUS LIPS — HZB, Institute Silicon Photovoltaics, Kekuléstr. 5, 12489 Berlin

The heterointerface between amorphous silicon (sub)oxides (a-SiO_x:H, 0<x<2) and crystalline silicon (c-Si) is investigated.

By varying SiH₄/CO₂ precursor gas mixtures, the stoichiometry of chemical-vapor-grown a-SiO_x:H layers was controlled, starting from pure a-Si:H to near-stoichiometric a-SiO₂. *In-system* photoelectron spectroscopy was employed to measure the valence band offset ΔE_V , while the defect density D_{it} , at the a-SiO_x/c-Si interface was determined using photoconduction decay.

We measure a systematic increase of ΔE_V starting from the established value of 0.3 eV for a-Si:H/c-Si to 4.3 eV for the a-SiO₂/c-Si heterojunction. Concomitantly the electronic quality (D_{it}) of the heterointerface deteriorates. For carrier transport across the a-SiO_x:H/c-Si heterojunction ΔE_V determines the barrier height for thermionic emission and/or tunneling of holes. Therefore the application of silicon suboxides in high-efficiency heterojunction solar cells seems to be unsuitable, mainly due to electronic transport hindrance resulting from the large ΔE_V , as also predicted by modeling studies [1].

The established analysis scheme can be readily applied to other types of heterojunctions, e.g. to promising silicon/metal oxide junctions [2].

[1] A. Kanevce et al., J. Appl. Phys. 105, 094507 (2009).

[2] C. Battaglia et al., Appl. Phys. Lett. 104, 113902 (2014).

HL 63.3 Thu 10:00 EW 015

Understanding 3C-SiC/SiO₂ interfaces in SiC-nanofiber based solar cells from *ab initio* theory — ●TAUFIK ADI NUGRAHA and STEFAN WIPPERMANN — Max-Planck-Institute for Iron Research, Düsseldorf, Germany

Nanostructured materials – such as e. g. hybrid nanocomposites consisting of inorganic semiconducting nanofibers and organic surfactants – provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized nanofibers can be performed completely using only inexpensive wet chemical solution processing. However, the synthesis conditions often lead to complex interfacial structures involving thin oxide layers between the nanofiber and surfactants, whose atomistic details are poorly understood at best. Here we present a combined density functional theory and tight binding investigation of interfaces between 3C-SiC nanofiber surfaces and SiO₂. Considering a wide variety of possible interfacial structures we utilize a grand canonical approach to generate a phase diagram and predict the structural details of the interface

as a function of the chemical potentials of Si, O and H. This study provides directions about how the synthesis conditions lead to specific types of interfacial structures and their impact on the electronic properties of the interface. The authors wish to thank U. Gerstmann, S. Greulich-Weber and W. G. Schmidt for helpful discussions. S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972.

HL 63.4 Thu 10:15 EW 015

Band offsets at the crystalline / hydrogenated amorphous silicon interface from first-principles — ●EBRAHIM HAZRATI, KAROL JAROLIMEK, and GILLES A. DE WIJS — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The heterojunction formed between crystalline silicon (c-Si) and hydrogenated amorphous silicon (a-Si:H) is a key component of a new type of high-efficiency silicon solar cell. Since a-Si:H has a larger band gap than c-Si, band offsets are formed at the interface. A band offset at the minority carrier band will mitigate recombination and lead to an increased efficiency.

Experimental values of band offsets scatter in a broad range. However, a recent meta-analysis of the results (W. van Sark et al. (Eds.): Physics & Tech. of Amorphous-Crystalline Heterostructure, pp. 405, Springer 2012) gives a larger valence offset (0.40 eV) than the conduction offset (0.15 eV).

In light of the conflicting reports our goal is to calculate the band offsets at the c-Si/a-Si:H interface from first-principles. We have prepared several atomistic models of the interface. The crystalline part is terminated with (111) surfaces on both sides. The amorphous structure is generated by simulating an annealing process at 1100 K, with DFT molecular dynamics. Once the atomistic model is ready it can be used to calculate the electronic structure of the interface. The position of band edges in the amorphous part is obtained by fitting the calculated density of states to a square root dependence. Our preliminary results show that the valence offset is larger than the conduction band offset.

HL 63.5 Thu 10:30 EW 015

Iron segregation at dislocations in silicon: a combined first-principles and kinetic Monte Carlo study — ●BENEDIKT ZIEBARTH^{1,2}, MATOUS MROVEC², CHRISTIAN ELSÄSSER², and PETER GUMBSCH^{1,2} — ¹Karlsruher Institute of Technology, Karlsruhe, Germany — ²Fraunhofer IWM, Freiburg, Germany

The efficiency of silicon based solar-cells is strongly affected by interstitial defects and impurities. Metallic impurities, in particular interstitial iron, result in a large loss of electric power production as they act as recombination centers for photo-induced charge carriers. It is known that metallic impurities like iron atoms are influenced by stress fields inside the silicon crystal. Here, we present a systematic study on how iron impurities are influenced by stress fields of dislocations in silicon using first-principles methods based on density functional theory. In a first step, the formation energies of iron impurities in bulk silicon has been investigated for hydrostatic, uniaxial and shear strain. Surprisingly, the most stable configuration of interstitial iron – the tetrahedral site – seems to be unaffected by any deformation of the crystal. Other configurations, however, are affected by deformations which results in a different diffusivity of Fe. The first-principles results from the formation energies are carried over to a kinetic Monte Carlo simulation in order to understand the effect on diffusion by a stress field induced by a screw dislocation or a 60° mixed dislocation. The kinetic Monte Carlo simulations reveal an effective segregation of iron atoms to the compressive-strain region of the mixed dislocation.

HL 63.6 Thu 10:45 EW 015

Structural and electrical properties of sulfur doped Si by ion implantation — ●FANG LIU^{1,2}, SŁAWOMIR PRUCNAL¹, KUN GAO^{1,2}, MUHAMMAD KHALID¹, WOLFGANG SKORUPA¹, MANFRED HELM^{1,2}, and SHENGQIANG ZHOU¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — ²Technische Universität Dresden, Dresden, Germany

Hydoping Si with chalcogens is one of the effective approaches to form an intermediate band (IB). This IB material is a candidate of infrared photodetectors and intermediate band solar cells. However, the chalcogens have relatively low solid solubility limit in Si. We prepared sulfur

doped silicon to above the Mott insulator concentration by ion implantation followed by pulsed laser annealing. The degree of crystalline lattice recovery in implanted layers and the lattice location of sulfur in Si were analyzed by Rutherford backscattering spectrometry / Channeling. Our results show that S atoms are occupying substitutional lattice sites in Si. We also observe an insulator-to-metal transition in silicon hyperdoped with sulfur to concentrations well above the maximum solubility limit of about $3 \cdot 10^{16} \text{ cm}^{-3}$. Analyzing temperature-dependent conductivity data, we find that a transition from insulating to metallic conduction occurs at a peak sulfur concentration of around $1 \cdot 10^{21} \text{ cm}^{-3}$.

HL 63.7 Thu 11:00 EW 015

Observation of Nitrogen Vacancy Center Fluorescence from Levitated Diamonds — ●ALEXANDER KUHLLICKE, ANDREAS W. SCHELL, JOACHIM ZOLL, HEATHER PARTNER, and OLIVER BENSON — Humboldt-Universität zu Berlin, Institut für Physik, AG Nanooptik, Newtonstraße 15, 12489 Berlin

Nitrogen vacancy (NV) defect centers in diamonds show remarkable optical properties and have emerged as perfect candidates for several different applications. Stabilization of diamond crystals in free space allows for particle isolation and is an important step towards optomechanical experiments on diamond nanoparticles. We report trapping of submicron diamonds in a linear quadrupole ion trap [1]. We discuss particle stability and the influence of surface charges, which are required for the electrodynamic confinement. The NV fluorescence of individual levitated clusters with diameters from micro- down to a few hundred nanometers can be observed. Optically characterized particles can be stored in the trap or deposited on photonic structures like fiber facets. Subsequently, an atomic force microscope can be used for

precise size measurements.

[1] A. Kuhlicke et al., Nitrogen vacancy center fluorescence from a submicron diamond cluster levitated in a linear quadrupole ion trap, Appl. Phys. Lett. 105, 073101 (2014)

HL 63.8 Thu 11:15 EW 015

A low-loss, broadband antenna for efficient photon collection from a coherent spin in diamond — ●DANIEL RIEDEL, DOMINIK ROHNER, MARC GANZHORN, TIMO KALDEWEY, PATRICK APPEL, ELKE NEU, RICHARD J. WARBURTON, and PATRICK MALETINSKY — Departement of Physics University of Basel, Basel, Switzerland

Light extraction from emitters in high-index, solid-state hosts is intrinsically difficult, but key to performance of applications in quantum-sensing, -metrology or -computing. We present a novel solution to this problem in form of a broadband, metal-free, low-loss optical antenna giving highly directed output for such emitters [1].

We engineer our device around individual nitrogen vacancy (NV) electronic spins in thin ($< 1 \mu\text{m}$), single-crystalline diamond membranes. We demonstrate the functionality of our antenna by measuring the emission patterns for different diamond layer thicknesses. Our findings show excellent agreement with an analytical theory and confirm that the NV emission is channeled preferentially into a medium-angle cone ($\text{NA} < 0.75$) in one direction. For broadband (640-750 nm), single NV fluorescence we report photon count rates approaching one MHz. Importantly, our photonic structure preserves the high spin coherence of NVs in single-crystalline diamond ($T_2 > 100 \mu\text{s}$).

Our results pave the way for near-unity photon collection efficiencies and unprecedented detection rates for not only NV centers, but a broad class of quantum emitters in high-index, solid-state systems.

[1] D. Riedel et al., accepted at Physical Review Applied