

O 99: Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Friday 10:30–12:45

Location: MA 042

O 99.1 Fri 10:30 MA 042

Surface and step conductivities at Si(111)-(7×7) surfaces investigated by multi-tip STM — ●SVEN JUST¹, MARCUS BLAB¹, STEFAN KORTE¹, VASILY CHEREPANOV¹, HELMUT SOLTNER², and BERT VOIGTLÄNDER¹ — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, and JARA-Fundamentals of Future Information Technology — ²Central Institute for Engineering, Electronics and Analytics (ZEA-1), Forschungszentrum Jülich

Four point measurements using a multi-tip scanning tunneling microscope (STM) are carried out to determine surface and step conductivities at Si(111)-(7×7) reconstructed surfaces. In a first step, distance dependent linear four point measurements are used to disentangle the 2D surface conductivity from bulk and space charge layer contributions. In order to further disentangle the surface conductivity of the step free surface from the contribution due to steps, the four probe method is applied in a quadratic configuration as function of the rotation angle. In total this combined approach allows to uniquely determine the surface conductivity, as well as the step conductivity at silicon surfaces.

O 99.2 Fri 10:45 MA 042

Atomic structure of terbium-induced nanostructures on Si(111) — ●MARTIN FRANZ, JAN GROSSE, ROBERT KOHLHAAS, and MARIO DÄHNE — Technische Universität Berlin, Institut für Festkörperphysik, Berlin

Rare earth metals are known to form a variety of very interesting self-assembled nanostructures on silicon surfaces. Examples are the metallic nanowires that form on the Si(001) and the Si(557) surface. On the planar Si(111) surface, the formation of two- and three-dimensional layers is observed.

Here, we report on a detailed scanning tunneling microscopy study on the growth and the atomic structure of terbium-induced nanostructures growing on the Si(111)7×7 surface for different terbium coverage. At extremely low coverage, the 7×7 substrate acts as a template for the growth of terbium-induced magic clusters. In the submonolayer regime, a $2\sqrt{3} \times 2\sqrt{3}$ superstructure, a chain-like 5×2 superstructure, and elongated islands with a 2×1 reconstruction on top are found. The 5×2 phase consists of alternating silicon Seiwatz and honeycomb chains with terbium rows in between. The observed different configurations can be explained by registry shifts between neighboring terbium rows or defects within one row. At higher coverage, the two-dimensional TbSi₂ monolayer forming a 1×1 reconstruction and the three-dimensional Tb₃Si₅ multilayer forming a $\sqrt{3} \times \sqrt{3}$ reconstruction are found.

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O 99.3 Fri 11:00 MA 042

Tailoring Si(100) substrate surfaces for GaP growth by Ga predeposition — ●MICHAEL HÄBERLE, BENJAMIN BORKENHAGEN, GERHARD LILIENKAMP, and WINFRIED DAUM — Clausthal University of Technology, Institute of Energy Research and Physical Technologies, Leibnizstraße 4, 38678 Clausthal-Zellerfeld, Germany

For GaP-on-Si(100) heteroepitaxy, currently considered as a model system for monolithic integration of III-V semiconductors on Si(100), the surface steps of Si(100) have a major impact on the quality of the GaP film. Monoatomic steps cause antiphase domains in GaP with detrimental electrical properties. A viable route is to grow the III-V epilayer on single-domain Si(100) with biatomic steps, but preferably not at the expense of reduced terrace widths introduced by miscut substrates [1]. We have performed in situ investigations of the influence of Ga deposition on the surface terrace dynamics of Si(100) at elevated substrate temperatures by low-energy electron microscopy (LEEM). Starting from nearly equally distributed T_A- and T_B-terraces of a two-domain Si(100) surface, submonolayer deposition of Ga resulted in a transformation into a surface with prevailing T_A-terraces. By increasing deposition rate or decreasing temperature, we induced restructuring of Si(100) into a surface dominated by T_B-terraces as reported by Hara et al. [2]. The occurrence and mutual transformations of surface structures with different terrace and step structures in a narrow range of temperatures and Ga deposition rates are discussed.

[1] K. Volz et al., J. Cryst. Growth 315, 37 (2011)

[2] S. Hara et al., J. Appl. Phys. 98, 083513 (2005)

O 99.4 Fri 11:15 MA 042

Calculated formation energies of charged defects at surfaces from the repeated-slab approach — ●CHRISTOPH FREYSOLDT and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Defects play an important role for the electrical, optical, and chemical properties of semiconductor surfaces under realistic conditions. In theory, the relevant structures, i.e., surfaces and point defects, are often simulated in the supercell approach. Yet, supercell calculations suffer from artificial interactions between the repeated images that are absent in the physical situation of interest. This is particularly problematic for formally charged defects because of the slow $1/r$ decay of the Coulomb interaction. In this contribution, we suggest a correction for the effect from an analysis of the underlying electrostatics. Screening is taken into account right from the beginning to account for potentially complex screening mechanisms. Yet, the universal long-range behavior limits the complexity to a finite range, allowing for simplified screening models in the end. By using a formulation based on charges and screened potentials, direct contact is made to electronic-structure calculations. The approach will be demonstrated for a model defect at the H-terminated Si(111) surface. The analysis reveals that the electric behavior of defects at surfaces depends on *two* macroscopic parameters (e.g. potential and field far from the surface), rather than *one* as for bulk point defects. Different choices of boundary conditions in charged surface calculations and extrapolation to arbitrary surface charges will be discussed.

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Nanoscale Structure of Si/SiO₂/Organic Interfaces — ●HANS-GEORG STEINRÜCK¹, ANDREAS SCHIENER¹, TORBEN SCHINDLER¹, JOHANNES WILL¹, ANDREAS MAGERL¹, OLEG KONOVALOV², GIOVANNI LI DESTRI², OLIVER H. SEECK³, MARKUS MEZGER⁴, JULIA HADDAD⁵, MOSHE DEUTSCH⁵, ANTONIO CHECCO⁶, and BENJAMIN M. OCKO⁶ — ¹FAU, Germany — ²ESRF, France — ³DESY, Germany — ⁴MPI Mainz, Germany — ⁵Bar-Ilan University, Israel — ⁶BNL, USA

Single-crystal silicon is by far the most widely used substrate for the deposition of organic thin films. It's surface is invariably terminated by a few nanometer-thick amorphous native SiO₂ layer. The structure of the transition layer between the silicon and it's oxide is neither well characterized nor well understood at present.

Using high-resolution x-ray reflectivity measurements of increasingly more complex interfaces involving silicon (001) substrates, we reveal the existence of a low-density, few-angstrom-thick, transition layer at the Si/SiO₂ interface [1]. The importance of accounting for this layer in modeling silicon/liquid interfaces and silicon-supported monolayers is demonstrated by comparing fits of reflectivity curves by models including this layer and the widely used Tidswell model [2], which excludes this layer. The 6-8 missing electrons per silicon unit cell area found here support previous theoretical models and simulations of the Si/SiO₂ interface [3].

[1] H.-G. Steinrück *et al.*, ACS Nano (2014), DOI: 10.1021/nn5056223.

[2] I. M. Tidswell *et al.*, Phys. Rev. B **41**, 1111 (1990).

[3] Y. Tu and J. Tersoff, Phys. Rev. Lett. **84**, 4393 (2000).

O 99.6 Fri 11:45 MA 042

Comparative study of Co and Ni germanides growth on Ge(001) substrates — ●TOMASZ GRZELA¹, WOJCIECH KOCZOROWSKI², GIOVANNI CAPELLINI^{1,3}, RYSZARD CZAJKA², NEIL CURSON^{4,5}, and THOMAS SCHROEDER^{1,6} — ¹IHP, Im Technologiepark 25, Frankfurt (Oder), 15236, Germany — ²Institute of Physics, PUT, Piotrowo 3, Poznan, Poland — ³Dipartimento di Scienze, Università degli Studi Roma Tre, Roma, Italy — ⁴London Centre for Nanotechnology, UCL, London, UK — ⁵Department of Electronic and Electrical Engineering, UCL, London, UK — ⁶BTU Cottbus, Konrad-Zuse Str. 1, 03046 Cottbus

Extending the performance of existing Si microelectronics beyond the limits faced by either miniaturization ("More Moore") or available functions ("More than Moore") requires the integration of new materials. Germanium, due to its superior physical properties with respect to Si in terms of optoelectronics and its CMOS processing compatibility, is one of the most promising materials to further develop the existing Si platform. However, there are challenges to the formation

of low resistance metallic contacts to Ge. Different metal/Ge systems present promising electrical properties, but given wide-spread use in Si CMOS technologies in form of their respective silicides-, cobalt- and nickel- germanides are of special importance. In this contribution we focus our attention on the systematic and comparative growth studies of Co- and Ni- germanides on Ge(001) substrates, by means of STM technique. In addition, other measurement technique like TEM-EDX, XPS and LEED were applied to corroborate these STM results.

O 99.7 Fri 12:00 MA 042

Investigation of the surface termination of BiTeI by combined STM/AFM — ●JULIAN BERWANGER, FLORIAN PIELMEIER, and FRANZ J. GIESSBL — Institut für Experimentelle und Angewandte Physik der Universität Regensburg, 93053 Regensburg, Deutschland

Cleaved BiTeI surfaces consist of domains which are either terminated by Te or I [1-3]. The size of these domains depends on the bulk crystallinity of the sample and ranges from 100 μm [1] to 100 nm [3]. The samples investigated here by a combination of scanning tunneling microscopy (STM) and atomic force microscopy (AFM) also consist of domains with smaller size. We find a similar surface structure as reported in Ref. 3 at 4.5K with plain STM in our room and low temperature STM/AFM experiments. Two different step heights are observed by STM in Ref. 3 and our experiments: 0.7 nm and 0.2 nm. The larger step height corresponds to the height of a -Bi-Te-I-stack. The smaller step height was also suggested to be a structural step caused by a stacking fault [3]. In contrast, the atomically resolved STM/AFM data of the smaller "step" suggests that this is indeed an atomically flat layer. The observed step height in STM is a purely electronic effect due to the different density of states at the Fermi-level of Te- and I-terminated surfaces. [1] Crepaldi et al. Phys. Rev. Letters 109, 096803 (2012) [2] Landolt et al. Phys. Rev. Letters 109, 116403 (2012) [3] Butler et al. Nat. Com. 5, 4066 (2014)

O 99.8 Fri 12:15 MA 042

Morphology of ultra-thin ZnO on Ag(111) — ●BJOERN BIENIEK¹, PATRICK RINKE^{1,2}, TAKASHI KUMAGAI¹, SHAMIL SHAIKHUTDINOV¹, BO HONG LIU¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz Haber Institut der MPG, Berlin, Germany — ²Aalto University, Helsinki, Finland

In the context of catalysis and hybrid inorganic/organic systems, metal supported ultra-thin ZnO can be used as model systems. However, the atomic morphology of these films is not well understood [1,2,3]. To in-

vestigate the thickness and termination of ZnO adsorbed on Ag we combine experimental techniques with all-electron density-functional theory calculations performed with the FHI-aims code and the PBE functional. PBE *ab initio* thermodynamics calculations predict H terminated 2×1-H structures to be most stable for all film thickness and H₂ pressures from low to ultra-high vacuum. However, a comparison of relative apparent height differences in calculated and measured scanning tunnelling microscopy (STM) images gives the best agreement for H- and OH-free two layer ZnO films. Further evidence for H- and OH-free unreconstructed ZnO films comes from the absence of OH peaks in infra-red spectroscopy and the comparison of measured and simulated field effect resonances (FER). We attribute this discrepancy to the *ab initio* thermodynamics prediction to kinetic effects such as energy barriers for the dissociation of H₂ and H₂O. [1] C. Tusche *et al.* PRL **99**, 026102 (2007) [2] Y. Martynova *et al.*, J. Cat., **301**, 227-223 (2013) [3] G. Weirum *et al.* J. Phys. Chem. C, 114 (2010)

O 99.9 Fri 12:30 MA 042

Adding 3D to conventional SEM or FIB surface imaging information - In situ Surface Sensing and Nanoprofilometry for Focused Electron and Ion Beam Induced Processes Verification — ●FRANK NOUVERTNE¹, AXEL RUDZINSKI¹, TORSTEN MICHAEL¹, MARC LEVERMANN¹, and EVA MAYNICKE^{2,3} — ¹Raith GmbH, Konrad-Adenauer-Allee 8, Dortmund, 44263, Germany — ²RWTH Aachen, 2. Phys. Inst., Otto-Blumenthal-Str. 28, 52074 Aachen, Germany — ³Klocke Nanotechnik GmbH, Pascalstr.17, 52076 Aachen, Germany

Recently, the bandwidth of nanofabrication applications for dedicated nanopatterning tools using Electron Beam Lithography (EBL) or FIB has significantly broadened. Some few latest generation professional and multi-technique electron and ion beam nanolithography tools even facilitate additional resistless, focused electron or ion beam induced in situ processes such as material deposition or gas enhanced etching. The number of variable parameters for such complex processes is nearly "infinite", so that an efficient in situ characterization of e.g. material deposition, milling or etching rates becomes crucial for most effective understanding and subsequent optimization of such processes.

We have implemented a nanomanipulator with nanoprofilometric capabilities, which allows efficient in situ characterization of nanostructures in 3D by collecting topographic sample surface information via line scans with approx. 10nm height resolution.

First results of direct in situ growth rate determination of focused electron beam induced material deposition (FEBID) will be presented.