O 10 Semiconductor surfaces and interfaces

Time: Monday 15:00–17:45 Room: PHY C213

O 10.1 Mon 15:00 PHY C213

Investigation of geometrical properties of NiMnSb-Half-Heusler thin films by X-ray reflectivity measurements. — •Andreas Stahl, Christian Kumpf, and Eberhard Umbach — Experimentelle Physik II, Universität Würzburg

The Half-Heusler alloy NiMnSb is an important material which may be utilized for the fabrication of spintronic devices due to it's unusual half-metallic properties. It can be grown in high crystalline quality on InGaAs/InP substrates, however, as for all heteroepitaxial systems mechanical stress is an important factor which influences crystalline quality, film growth, and magnetic properties. One example is a magnetic anisotropy which depends on the thickness of the Half-Heusler layer [1].

We present a series of x-ray reflectivity measurements on MBE-grown NiMnSb thin films from 10nm to 200nm thickness. Some of the samples were capped with an amorphous Au/Ti layer in order to avoid oxidation in air. The reflectivity scans were performed at the six-circle-diffractometer at BW2, HASYLAB, Hamburg. We discuss important parameters like the layer thicknesses, the roughnesses of the interfaces and the electron densities of the Half-Heusler layers [2].

[1] A. Koveshnikov et al.: J. Appl. Phys. \textbf{97}, 073906 (2005).
[2] A. Stahl et el.: to be published.

O 10.2 Mon 15:15 PHY C213

Morphology of ultrathin manganese silicide films on Si(001) and Si(111) substrates — •Mahbube Hortamani, Peter Kratzer, and Matthias Scheffler — Fritz-Haber Institut, Faraday weg 4-6, 14195 Berlin, Germany

Recently, the field of spintronics has attracted much attention since it provides knowledge for a novel type of electronic devices that use the electron's spin, in addition to its charge, for processing and storage of data. Ferromagnetic metal/semiconductor interfaces hold great promise for fabrication of such devices. Covering Si with a layer of Mn intermetallic compounds is one possibility to produce such interfaces. We investigate the stability of Mn_xSi_y films on Si for various stoichiometries and atomic structures of the films, using density functional theory with the GGA-PBE functional and the FP-APW+lo method. We find that for ultrathin film growth on the Si substrate, the manganese-silicon multilayers with 1:1 stoichiometry (MnSi) are more stable than a pure Mn film or other silicide compounds. The formation of the B20 structure on the Si(111) substrate is found to be thermodynamically more stable than films of other structures. While the B20 structure is not compatible with the Si(001), we suggest a closly lattice-matched B2 structure to form on this surface. By simulating the proposed B2 structure on both (001) and (111) surfaces, we find that the film formation on Si(111) is energetically favorable. However, the films on Si(001) are metastable compared to formation of MnSi islands, and hence Volmer-Weber growth is expected. In all MnSi films on Si(111) the Mn atoms in the interface and surface layer have sizable magnetic moments.

O 10.3 Mon 15:30 PHY C213

In/Si(111): Chain structure and metal-insulator transition — •Andrey Stekolnikov, Jürgen Furthmüller, and Friedhelm Bechstedt — Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, D-07743 Jena

Atomic geometry and electronic structure of quasi-one-dimensional (1D) In/Si(111) systems with 4×1, 4×2, and 8×2 translational symmetries are studied by means of *ab-initio* calculations. While the 4×1 structure shows metallic behavior, the 4×2 (8×2) reconstruction leads to a pure semiconducting phase. For 4×2 (8×2) reduction of the total energy and formation of the energy gap are related to an additional bonding within the double In zig-zag chains. Simulated STM images show a good agreement with experimental ones. The geometry of In chains is very sensitive to all possible interactions. Several local minima may occur on the total-energy surface. The description of In-In and In-Si bonds plays an important role. The influence of the exchange and correlation within density functional theory calculations as well as In *d*-electrons is discussed in detail.

O 10.4 Mon 15:45 PHY C213

Optical properties of the Si(113) 3×2 ADI surface — •Katalin Gaal-Nagy — Dipartimento di Fisica, Universita degli Studi di Milano, Via Celoria 16, 20133 Milano (Italy)

We have investigated the optical properties of the 3×2 ADI reconstruction which is the most stable structure of the (113) surface of silicon. The calculations have been done within the plane-wave pseudopotential approach to the density-functional theory as implemented in ABINIT [1] and TOSCA [2]. Besides, also a semi-empirical tight-binding approach has been used. In a first step, tests on the atomic geometry, the slab thickness, and the electronic structure have been performed. The optical properties have been derived using the matrix elements of the momentum operator through the calculation of the x and y contribution to the imaginary part of the polarizability, from which the RAS (reflectance anisitropy spectra) can be obtained. With a layer-by-layer analysis the surface contributions have been disentangled from the ones of the bulk-part of the slab. Finally, we compare our results with available theoretical and experimental data.

[1] http://www.abinit.org
[2] http://users.unimi.it/etsf/tosca.html

O 10.5 Mon 16:00 PHY C213

Investigation of the System Hafnium/Silicon(100) by means of XPS and X-ray Photoelectron Diffraction (XPD) — •C. Fluechter[1,2], D. Weier[1,2], S. Dreiner[1], M. Schürmann[1], U. Berges[1,2], M.F. Carazzolne[3], A. de Siervo[3,4], R. Landers[3,4], G.G. Kleiman[4], C. Westphal[1,2], and E. Henschel[1] — [1]Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - Universität Dortmund, Maria-Göppert-Meier-Str. 2, D 44227 Dortmund, Germany — [3]Laboratório Nacional de Luz Sincrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — [4]Instituto de Fisica - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

The ongoing miniaturization of transistor devices in the semiconductor industry calls for a new gate dielectric, replacing silicon oxide (SiO_2) that has been used for decades. One of the candidates, i.e. hafnium oxide (HfO_2), is investigated in this work by studying ultrathin films of the pre system HfSi/Si(100) via XPS, LEED and Photoelectron Diffraction with a magnesium x-ray source. Several heating curves are presented showing that, unlike for thick layers, no phase transitions of the ordered HfSi films can be observed. Also, an island formation of the annealed film is indicated. Simulations of the structure of the system are shown and compared to experimental diffraction pattterns. We propose a possible interface structure for Hf/Si(100) to bulk Si. Finally, possibilities for oxidizing and transforming the prepared HfSi into HfO_2 are introduced.

O 10.6 Mon 16:15 PHY C213

Photothermal patterning of H-terminated silicon substrates: Writing nanostructures with a micron-sized laser beam — •Rafael Bautista, Thorsten Balgar, Steffen Franzka, Nils Hartmann, and Eckart Hasselbrink — Universität Duisburg-Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

A focused beam of an argon ion laser at a wavelength of 514 nm is used for rapid large-area patterning of H-terminated Si(100) substrates under ambient conditions [1]. The technique allows for the preparation of well-confined, ultrathin oxide structures with a lateral dimension significantly below the diffraction limited laser spot diameter of the optical setup. In particular, at a focal spot diameter of about 2.5 μm oxide lines with a width from several microns down to 300 nm are prepared. At even smaller spot diameters structures with a lateral dimension below 200 nm are reached. The patterning experiments under ambient conditions are complemented by investigations in an ultrahigh vacuum environment. A simple thermokinetic analysis of the data allows to estimate effective kinetic parameters of the patterning process and reproduce the experimentally observed functional dependence of the line width on the incident laser power and the writing speed. The underlying highly superlinear dependence of the overall patterning process on the laser intensity is traced back to the interplay between the laser-induced transient local temperature rise and the thermally activated hydrogen desorption.

[1] T. Balgar, S. Franzka, N. Hartmann, E. Hasselbrink, Langmuir 20

(2004) 3525.

O 10.7 Mon 16:30 PHY C213

Photothermally induced dehydroxylation on surface-oxidized silicon substrates: A simple means for the fabrication of submicron-structured hydrophilic/hydrophobic templates — •Nils Hartmann, Thorsten Balgar, Steffen Franzka, and Eckart Hasselbrink — Universität Duisburg-Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Patterns with alternating hydrophilic and hydrophobic domains are widely used to control and study processes at surfaces in many fields of material science. We recently reported a laser-assisted procedure for the fabrication of hydrophobic patterns on hydrophilic, surface-oxidized silicon substrates [1]. Local irradiation with a highly focused laser beam at a wavelength of 514 nm results in photothermal dehydroxylation and converts the affected surface areas from hydrophilic to hydrophobic. The patterns are stable for weeks or longer, even if the samples are stored at ambient conditions. Contrary to ordinary avenues to hydrophilic/hydrophobic patterns no coating is required. This makes the procedure extremely simple and robust. Routine patterning can be carried out over large areas at fast writing speeds under ambient conditions. At a focal spot diameter of about 2.5 μm, hydrophobic lines with a width down to 0.4 μm are prepared. The laterally varying hydrophilicity provides an opportunity to further functionalize the surface. In particular, as shown here, the patterned substrates represent suitable templates for the directed self-assembly of organic monolayers.

[1] T. Balgar, S. Franzka, E. Hasselbrink, N. Hartmann, Appl. Phys. A, in press.

O 10.8 Mon 16:45 PHY C213

Sum-frequency generation study of hydrogen diffusion on vicinal Si(100) surfaces induced by resonant IR laser excitation — •Xu Han, Kristian Lass, and Eckart Hasselbrink — Fachbereich Chemie, Physikalische Chemie, Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

We report first measurements of a new way (non-thermal, non-electronic excitation) of inducing adatom diffusion. Under selective resonant excitation by tunable IR laser pulses, hydrogen diffusion between step sites or from step edges onto terraces of a vicinal Si(100) surface has been demonstrated. The state of the adsorbate has been monitored by means of IR-visible sum-frequency generation spectroscopy (using ps laser pulses). Hydrogen preferentially binds to the step edges on a Si(100) surface with D_B or S_B steps. For saturation coverage the stretch vibration of step-bonded monohydrides has been found at 2087 cm^{-1}, with a small blue shift at lower coverages. Hydrogen diffusion from D_B or S_B step edges to other weakly bonded sites at steps can be enhanced by resonant IR laser excitation at temperatures well below the threshold for thermally activated surface diffusion of hydrogen. Alternatively, hydrogen can also diffuse onto terraces, where the frequencies of isolated monohydride, monohydride with neighboring dihydride, and dihydride are 2100, 2104 and 2107 cm^{-1}, respectively, with a small red shift at lower coverages.

O 10.9 Mon 17:00 PHY C213

MOMBE growth of ZnO on SiC - a photoemission study — •Stefan Andres[1], Christian Pettenkofer[1], and Thomas Seyller[2] — [1]Hahn-Meitner-Institut, Glienicker Str. 100,D-14109 Berlin, Germany — [2]Institut of Technical Physics, University of Erlangen, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Zinc oxide (ZnO) is a semiconductor with a direct band gap of 3.3eV and therefore an interesting candidate for future applications in the area of opto-electronics in the UV regime or transparent electronics.

We report on the growth of thin ZnO films on 6H-SiC(0001) substrates. The films were grown using Metal Organic Molecular Beam Epitaxy (MOMBE). Changes in surface morphology and electronic structure during film growth were investigated by low energy electron diffraction (LEED) and photoelectron spectroscopy (PES), respectively. The qualitative LEED images show that highly oriented ZnO(0001) films are formed. However, facceting of the surface is observed during the initial stages of ZnO growth and also beyond the monolayer coverage. A careful quantitative and qualitative examination of the SiC and ZnO core and valence band levels reveals the growth mode to be of the Frank v.d. Merwe type. Furthermore, we will comment on the the band alignment of the SiC/ZnO interface.

O 10.10 Mon 17:15 PHY C213

RF-sputtered indium-tin-oxynitride films investigated by photoelectron spectroscopy — •Marcel Himmerlich[1], Maria Koufaki[2], Manolis Sifakis[2], Stefan Krischok[1], Elias Aperathitis[2], and Juergen A. Schaefer[1] — [1]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Microelectronics Research Group, IESL, Foundation for Research & Technology–HELLAS, P.O. Box 1527, 71110 Heraklion, Crete, Greece

Indium-tin-oxide (ITO) and indium-tin-oxynitride (ITON) thin films have been fabricated by rf-sputtering in Ar or N_2 plasma, respectively. The deposition was performed on pre-cleaned Si using an ITO target (80% In_2O_3 + 20% SnO_2). During the growth procedure the gas flow was controlled to maintain a total pressure of 5×10^{-3} Torr in the chamber. The dependence of the surface chemical composition and the electronic properties on the rf power were examined using photoelectron spectroscopy (XPS, UPS). Changes upon annealing were investigated by rapid thermal annealing in N_2 atmosphere as well as by in vacuo heating combined with a monitoring of the gas desorption using a quadrupole mass spectrometer. The observed differences in the carrier concentration are well correlated with the existence or absence of an oxygen reduced phase in the films, as can be seen by a high binding energy feature in the O1s, Sn3d and In3d core levels. A complex incorporation of nitrogen into the ITON films was found which reveals itself in the existence of 5 different N1s states. Annealing above 550°C resulted in a release of nitrogen combined with the formation of the oxygen reduced phase.

O 10.11 Mon 17:30 PHY C213

XPS and XPD studies on the system Hafnium(oxide) on Si(100) using soft x-rays — •D. Weier[1,2], C. Flüchter[1,2], S. Dreiner[1], M. Schürmann[1], U. Berges[1,2], M.F. Carazzolne[3], A. Pancotti[3], R. Landers[3,4], G.G. Kleiman[4], C. Westphal[1,2], and E. Henschel[1] — [1]Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - Universität Dortmund, Maria-Göppert-Meier-Str. 2, D 44227 Dortmund, Germany — [3]Laboratório Nacional de Luz Sincrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — [4]Instituto de Fisica - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

Continuous down-scaling of the silicon based MOSFETs results in gate lengths of less than 100 nm. Scaling down the gate dielectric to less than 15 $\AA$ is not possible using SiO_2 because of an increasing leakage current. Presently, there are many higk-k candidates discussed as a substitution for SiO_2 as the gate dielectric. One of the most promising candidates is HfO_2. In this work ultrathin films of HfSi on Si(100) were studied by XPD to investigate possible interface structures between Silicon and Hafnium. It will be shown that a modified C49 structure is found for HfSi by a comparision of experimental with simulated diffraction patterns. Further on, experimental XPS and XPD results for the systems HfO/Si(100) are shown.