O 13: Semiconductor substrates: Adsorption

Time: Monday 15:00–17:45 Location: H34

O 13.1 Mon 15:00 H34

metallic transport and Anderson localization on In atomic layers on silicon — •Shiro Yamazaki[1], Yoshikazu Hosomura[2], Iwao Matsuda[3], Rei Hobara[2], Toyoaki Eguchi[3], Yukio Hasegawa[3], and Shuji Hasegawa[2] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics, The University of Tokyo, Tokyo, Japan — [3]The Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan

Metallic electrical transport have not been observed in atomic-scale low-dimensional metal systems at low temperature region due to Anderson localization effect, except to Graphene or extremely conductive polyaniline [1,2]. Si(111)-$\sqrt{7} \times \sqrt{3}$-In surface reconstruction is a In atomic layer supported by Si(111) substrate. According to ARPES study, the surface shows 2D metal state with the very large Fermi wave number (k_F=14[nm^{-1}]) and the large electron density (4.6$\times$10^{14} [eV^{-1} cm^{-2}]) [3], leading to a low resistance. By using variable-temperature micro-four-point probe method [3], very low resistance and metallic transport was found down to 10 K. It is quantitatively explained by the ARPES result by using 2D Boltzmann equation $R_{2D} = \frac{4\pi^2 \lambda m^*}{e^2 \hbar k_F^2} k_B T$. By introducing defects, it shows semiconducting temperature dependence of variable range hopping due to Anderson localization. [1]K. S. Novoselov, et al. , Nature **438**, 197 (2005) [2]K. Lee, et al. , Nature **441**, 65 (2006) [3]E. Rotenberg, et al. , Phys. Rev. Lett. **91**, 246404 (2003) [4]T. Tanikawa, et al. , e-J. Surf. Sci. Nanotech. **1**, 50 (2003)

O 13.2 Mon 15:15 H34

Thermal stability of ultra-thin ZrO_2 films and structure determination of $ZrSi_2$ islands on Si(100) — •Frank Schönbohm[1,2], Christian Rolf Flüchter[1], Daniel Weier[1], Tobias Lühr[1], Ulf Berges[1,2], Sven Döring[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Technische Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund, Germany

The ongoing miniaturisation of semiconductors requires a substitute for the presently used SiO_2 gate dielectrics. Below 2 nm film thickness the leakage current increases drastically due to tunneling processes and causes the loss of efficiency. Among the *high-k* materials HfO_2 and ZrO_2 might be proper candidates to replace the SiO_2. We studied the temperature dependence of thin ZrO_2 films on clean silicon by means of x-ray photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD). ZrO_2 films with a thickness of approximately 11 Å were grown by electron beam evaporation on a (2×1)-reconstructed Si(100) surface. At annealing temperatures of 650°C and above the ZrO_2 films were transformed into $ZrSi_2$. The temperature region of structural transformation could be narrowed to the range from 650°C to 725°C. During the formation of $ZrSi_2$ all oxygen was removed from the sample surface. After annealing at 725°C neither zirconia nor silicon oxide could be verified on the sample. From the combined spectroscopy, SEM, and XPD analysis a model for the internal structure of $ZrSi_2$ is proposed.

O 13.3 Mon 15:30 H34

Characterization of Si(112) and In/Si(112) studied by SPA-LEED — •Jan Höcker, Moritz Speckmann, Thomas Schmidt, and Jens Falta — Institute of Solid State Physics, University of Bremen, 28359 Bremen

High index surfaces are of strong interest in todays research because of the possibility to grow low dimensional structures. It has for instance already been shown that the adsorption of Ga can induce the formation of 1D metal chains on Si(112) (cf. Snijders et al., PRB **72**, 2005). In this work we investigated the clean Si(112) surface and the adsorption of In on Si(112) to establish an analogy to Ga/Si(112) using spot profile analyzing low energy electron diffraction (SPA-LEED).

By means of reciprocal space mapping we determined the bare Si(112) surface to be decomposed into alternating (5 5 12) and (111) facets in $[1\bar{1}0]$ direction with (2×1) and (7×7) reconstruction, respectively (cf. Baski et al., Surf. Sci. **392**, 1997).

With SPA-LEED we were able to observe the decreasing intensity of the facet spots in-situ while depositing In on Si(112) and thus reveal the smoothening of the surface due to the deposition of In. At saturation coverage we found a "$(3.x \times 1)$" reconstruction, where x is dependent on the deposition temperature and changes from $x = 7$ at 400°C to $x = 5$ at 500°C. This leads us to the assumption that the reconstruction is not incommensurate but a mixture of (3×1) and (4×1) building blocks, which is very similar to the super structure of Ga on Si(112).

O 13.4 Mon 15:45 H34

Adsorption of metalorganic molecules on metal-semiconductor systems — •Jędrzej Schmeidel, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Abteilung Atomare und Molekulare Strukturen, Appelstrasse 2, 30167 Hannover, Germany

Molecular junctions appropriate for transport trough single molecules can be realized using concepts of surface science. The controlled opening of ultra-thin Ag nanostructures on Si surfaces by electromigration and injection of single ferrocene molecules has been demonstrated recently [1]. In order to model accurately the conductivity of ferrocene-1,1'-dithiol molecules, thiolate bounded molecules are adsorbed on perfect sites of the Ag contacts. However, chemisorption takes place at defect sites, e.g. atomic step [2]. For an detailed understanding of this complex scenario we have investigated the adsorption of metal organic molecules on metal/semiconductor surfaces. As substrate the Ag $\sqrt{3}$ reconstruction, Ag islands and Ag multilayers on Si(111) have been investigated by means of STM and STS. Only without the wetting layer, Ag nanostructures can be electronically decoupled from the substrate as seen by a Coulomb blockade oscillations of the double barrier structure [3]. In order to study the selectivity of defects regarding molecular adsorption, porphyrins and ferrocene-1,1'-dithiol molecules have been adsorbed on these structures. The molecules adsorb predominantly at defects sites, e.g. steps and grain boundaries, as observed in the bias dependence of the STM image contrast.
[1] APL 89, 063120, [2] JCP 128, 064704, [3] PRB 80, 115304

O 13.5 Mon 16:00 H34

Comparison on the local adsorption of pyridine and cyclopentene on Si(100) — •Daniel Weier[1,2], Tobias Lühr[1], Frank Schöhnboh[1,2], Axel Beimborn[1], Max Brucker[2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

We investigated the chemical and geometrical properties of the systems pyridine on Si(100) and cyclopentene on Si(100) in a combined of photoelectron spectroscopy (XPS) and photoelectron diffraction (XPD) study. The experiment had been performed by applying synchrotron radiation in order to achieve a high resolution with high surface sensitivity. Our XPS and XPD results show that cyclopentene reacts with one silicon-dimer of the (2x1)-reconstructed surface in a [2+2]-cycloaddition, changing the planar molecule to a diverse tilted molecule after adsorption. The pyridine contrariwise reacts with two of the silicon dimers by a combined reaction of cycloaddition and Lewis-acid base reaction. We will provide and compare structure models for both systems including detailed structure parameters obtained within a comprehensive numerical analysis.

O 13.6 Mon 16:15 H34

Structural study of self-assembled Lead-Phthalocyanine ultra-thin layers on GaAs(001) — •Linda Riele[1,2], Benjamin Buick[1], Thomas Bruhn[2,3], Eugen Speiser[1,3], Bjørn-Ove Fimland[4], Michael Kneissl[2], Norbert Esser[2,3], Patrick Vogt[2], and Wolfgang Richter[1] — [1]Università di Roma Tor Vergata, Rome, Italy — [2]TU Berlin, Berlin, Germany — [3]ISAS Department Berlin, Berlin, Germany — [4]Dept. of Electronics and Telecommunications, NTNU, Trondheim, Norway

Phthalocyanine molecules attract a growing scientific and technological interest because of their potential use for sensing applications. A systematic design of devices based on heterostructures, however, requires a profound understanding and control of the structural and electronic properties of organic/inorganic interfaces. Here we report on the non-planar lead phthalocyanine (PbPc) layers deposited on GaAs(001) with c(4×4), (2×4) and (4×2) reconstructed surfaces. The samples were investigated with Raman spectroscopy, reflectance anisotropy spectroscopy (RAS) and scanning tunneling microscopy (STM). RAS revealed a strong influence of the initial GaAs(001) surface reconstruction on the molecular arrangement within 20 nm thick PbPc films. Structural differences could also be verified by Raman spectra showing significant differences (frequencies, intensities and angular dependency). Moreover, STM measurements elucidated the influence of the GaAs substrate surface reconstructions on the organic film structure within the first monolayer.

O 13.7 Mon 16:30 H34

Adsorption of PTCDA on GaN(0001) surfaces — •Christian Schulz[1], Cherno Jaye[2], Christian Tessarek[1], Stephan Figge[1], Jan Ingo Flege[1], Thomas Schmidt[1], Detlef Hommel[1], Daniel A. Fischer[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Ceramics Division, National Institute of Standards and Technology, Gaithersburg, MD 20899

Ordered growth of thin PTCDA layers is mainly observed on metals but recent reports (S. Yim et al. *J. Phys.: Condens. Matter* **15**, (2003)) have shown that some molecules also show ordered layers on unpassivated III-V semiconductor surfaces. In this work we investigate the adsorption of PTCDA on gallium-polar GaN(0001) with different methods. X-ray photoelectron spectroscopy (XPS) shows that the molecules are not dissociating after deposition, because the peak area ratios (including the shake-up's) for the perylene to carboxylic C1s feature is near the expected ratio for the intact molecule. Scanning tunneling microscopy (STM) and spot profile analyzing low energy electron diffraction (SPA-LEED) measurements reveal an island growth mode. For monolayer equivalent deposits, the near edge X-ray absorption fine structure (NEAFS) data of the C K-edge exhibit no polarization dependence indicating a disordered mixture of molecules in upstanding and down-lying geometry. However, for multilayer equivalent deposits a polarization dependence is observed which suggests a flat-lying geometry of the molecules. These findings are in good agreement with high-resolution STM and SPA-LEED data which reveal lateral ordering, compatible with a bulk-like configuration, within the islands.

O 13.8 Mon 16:45 H34

SHG Spectroscopy of Potassium-Covered Si(100)(2x1) — •Dominic Gerlach, Björn Braunschweig, Gerhard Lilienkamp und Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

Previous second-harmonic generation (SHG) studies of potassium-modified Si(100)/SiO2 interfaces have revealed dramatic changes in the SHG spectra due to the presence of potassium ions at the interface and electric-field-induced second-harmonic generation in the space charge region of the semiconductor [1]. Here we present results of SHG experiments with a saturation layer of potassium (0.5 monolayer) deposited on clean Si(100)(2x1) surfaces. The main effect of the potassium adlayer on the SHG spectrum is a spectrally flat background contribution similar to a metal surface. The strength of the surface E1 resonance of the undoped Si substrate is almost unaffected by the adlayer, although it appears strongly enhanced in the spectra by interference. An additional resonance at 3.9 eV is tentatively assigned to a surface plasmon excitation in the potassium layer. The SHG results are consistent with a metallic character of the adsorbed potassium.

[1] A. Rumpel et al., Phys. Rev. B 74 081303(R) (2006)

O 13.9 Mon 17:00 H34

Potential energy diagram for the selective adsorption of C_{60} on Bi terminated Si and Ge surfaces — •Vasily Cherepanov[1], Stefan Korte[1], Sergey Filimonov[2], and Bert Voigtländer[1] — [1]Institute of Bio and Nanosystems (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Department of Physics, Tomsk State University, Tomsk 634050, Russia

Si/Ge nanostructures can be grown using a surfactant like Bi in order to suppress Si-Ge intermixing. Choosing appropriate growth conditions one can achieve a chemical selectivity for C_{60} adsorption and C_{60} adsorbs only onto the Ge area of the surface. A passivation of dangling bonds on Si and Ge surfaces by Bi atoms results in an adsorption of C_{60} molecules on top of Bi layer in a physisorbed state. At elevated temperatures the deposited C_{60} molecules desorb from the physisorbed state back to the gas phase or transfer to a chemisorbed state by substituting Bi and bonding directly to the substrate. The C_{60} molecules in physisorbed and chemisorbed state can be easily distinguished in Scanning Tunneling Microscopy images. Measurements of the temperature and rate dependences of the density of C_{60} molecules in physisorbed/chemisorbed state allow to plot the potential energy diagram for adsorption of C_{60} on Bi terminated Si and Ge surfaces. The knowledge of the adsorption diagrams for Si and Ge is essential to choose the proper growth condition for selective adsorption and thereby to achieve a desired functionality of the surface.

O 13.10 Mon 17:15 H34

First-principles study of H diffusion on Si(001) — •Jürgen Wieferink[1,2], Peter Krüger[1], and Johannes Pollmann[1] — [1]Institut für Festkörpertheorie, Universität Münster — [2]Fritz-Haber-Institut, Berlin

Hydrogen diffusion on the Si(001)-(2×1) surface is crucial for an understanding of molecular H_2 desorption. On flat Si(001) terraces, only diffusion along the dimer rows is found for moderate temperatures and low H coverage. On the other hand, the occurrence of vacancy interrow transitions on a monohydride surface has been demonstrated by a recent study combining pulsed laser heating and scanning tunneling microscopy (STM) [1].

After a general introduction of the experimental findings we will present the results of our ab initio study on activation energies and diffusion rates as function of H coverage. The barrier energies depend strongly on the distance between the Si atoms in the transition state. As the monohydride surface is more rigid than the clean surface, isolated vacancies are less mobile than isolated H atoms. Interestingly, two adjacent vacancies may transfer charge from one to another prior to a vacancy transition, which significantly lowers the barrier.

[1] C. H. Schwalb, M. Dürr, U. Höfer, *Phys. Rev. B* **80**, 085317 (2009).

O 13.11 Mon 17:30 H34

Self-assembly of aromatic heterocyclic molecules on GaAs surfaces — •Thomas Bruhn[1,2], Bjørn Ove Fimland[3], Michael Kneissl[1], Norbert Esser[1,2], and Patrick Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [3]NTNU, NO-7491 Trondheim, Norway

Although organic/inorganic interfaces are already used in a variety of technological applications, such as OLEDs or sensors, there is still no sufficient basic understanding of the structural and electronic parameters that influence the interface formation between the organic and the inorganic material. We investigate organic adsorbates on technologically important III-V surfaces. After having gained detailed understanding of the adsorption of unsaturated hydrocarbon ring molecules, we investigate the adsorption of the aromatic heterocyclic molecule Pyrrole (C_4H_4NH) on clean GaAs(001) surface reconstructions. The samples were prepared under UHV conditions and the adsorption process was monitored in-situ with reflectance anisotropy spectroscopy (RAS). The interfaces were characterized electronically by scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and photoemission spectroscopy (PES). The measurements show a significantly higher surface reactivity for the Ga rich surface reconstructions and indicate a physisorption of the adsorbed molecules at the As-rich $c(4 \times 4)$ reconstruction. Intra-molecular bondings could be identified in the tunneling spectra and molecular adsorption sites could be determined from the STM measurements.