

International workshop on

LEED and related techniques



Hannover 28-29 May 2015

organized by the Institute of Solid State Physics Leibniz University of Hannover

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Heike Kahrs, Herbert Pfnür, Christoph Tegenkamp Institut für Festkörperphysik, Leibniz Universität Hannover Appelstrasse 2 30167 Hannover, Germany Venue: Multimedia Hörsaal, Applestrasse 4, 39167 Hannover This SPA-LEED workshop is supported by:





SP€CS[™]



Laboratory of Nano and Quantum Engineering

Coffee breaks & Meals

- Lunch on Thursday 28th May is served in the **Mensa**, Callinstraße.
- Lunch on Friday, 29th May is served next to the lecture hall (room 023)
- During the breaks coffee, tea, fruits and biscuits will be served next to the lecture hall
- During the poster session on Thursday in the LNQE beer and pretzels are served
- Thursday evening: Buffet-style dinner (including meals for vegetarians) is served in the restaurant **Zwischenzeit** (Schaufelderstr.11) (please note that alcoholic drinks are not included)

Internet access at the venue

To access the wireless LAN service, please connect either to the "eduroam" or the "LUHWPA" network. For the "LUHWPA" access point please ask for login data at the reception desk.

Venue

<u>Talks:</u> Multimedia Hörsaal, Room 023, Appelstr. 4, 30167 Hannover <u>Posters:</u> Laboratory for Nano- and Quantenengineering (LNQE), Schneiderberg 39, 30167 Hannover

emergency No. 🕾 +49 (0)176-28371883 (Christoph Tegenkamp, mobile)

Map of the conference site:

<u>| 30 m |</u> 100 ft |

(Conference room - Poster session - Mensa - conference dinner)



Program Overview

Thursday,	28 May 2015	
9:00		Reception open
9:15		Opening remarks
9:30-10:10	Ed Conrad (invited)	The role of structural information in the progress towards semiconducting graphene
10:10-10:40	Stefan Heun	Correlation between Morphology and Transport Properties of Quasi-Free- Standing Monolayer Graphene
10:40-11:20	Coffee break	
11:20-12:00	Shuji Hasegawa (invited)	Surface transport below 1 K
12:00-12:30	Michael Horn-von Hoegen	Electron Diffraction at Surfaces: by now Ultrafast!
12:30-14:00	Lunch (Mensa)	
14:00-14:40	Georg Held (invited)	Challenges and Prospects of Surface Crystallography by LEED
14:40-15:10	Jan Ingo Flege	Low-energy electron microscopy and micro-diffraction analysis of nanoscale transient cerium oxide phases during reduction by molecular hydrogen
15:10-15:40	Lutz Hammer	Crystallographic analysis of one- dimensional metal and metal-oxide hybrid structures formed on the Ir(100) surface
15:40-16:00	Coffee break	
16:00-19:00		Poster session / LNQE Building
From 19:30		Conference Dinner / Zwischenzeit

Friday,	29 May 2015		
8:45		Reception open	
9:00-9:40	Moritz Sokolowski (invited)	SPA-LEED and high resolution optical spectroscopy of molecules on surfaces	
9:40-10:10	Christian Teichert	Facet analysis using Atomic Force Microscopy	
10:05-10:30	Arie van Houselt	Au/Ge(001): a wetting-dewetting transition	
10:30-11:30		Coffee break & Champagne reception	
11:30-11:50	Grußworte des Dekans, Prof. Dr. Uwe Morger		
	Musikalische Untermalung durch Gerd-Harald Knauf, Klavier & Herbert Pfnür, Violoncello:		
	Franz Schubert: aus Sonate a-moll D821, Adagio, Allegretto Camille Saint-Saens: Allegro appassionato op.43		
11:50-12:30	Ceremonial talk: Hans Lüth (invited)	Surface Science: Historical Remarks and Martin Henzler's Role	
12:30		Lunch buffet	
14:00		Lab tours	

The role of structural information in the progress towards semiconducting graphene

Edward H. Conrad Georgia Institute of Technology, Atlanta, GA, USA

Since the inception of graphene research, the goal has been to use this 2D material for next generation electronics. The vast majority of the research since 2001 has focused on exfoliated graphene produced by various methods and transferred to a suitable substrate. This field has had little impact on graphene electronics, leading the National Science Foundation to limit funding for graphene and instead focus on other 2D materials that are even more difficult to grow. What is ironic is that this decision is based on very little information about graphene. The lack of information is simply due to the fact that exfoliated graphene is highly disordered. This makes employing almost all traditional surface science probes nearly impossible; a situation particularly distressful for a pure 2D system. Producing and studying ordered graphene is essential to any future progress. Furthermore, once it is understood that isolated graphene does not exist, it is critical that we understand the substrate-graphene interaction to make any substantive progress towards graphene electronics. In this talk I will focus on highly ordered epitaxial graphene grown on the SiC(0001) surface. Recent advances in material growth has led to new discoveries about this form of graphene including exceptional ballistic transport in graphene ribbons and the discovery of a wide band semiconducting form of graphene. I will talk about two works; graphene grown on the sidewalls of SiC steps and new work showing that the first graphene layer is a true semiconductor.

Graphene grown on sidewalls of trenches shows ballistic transport, exceptional mobilities, low intrinsic doping, and the opening of a band gap. While early theoretical work predicted a band gap in graphene ribbons depending on one of the two types of edge terminations ("armchair" and "zigzag"), it was never experimentally verification because of edge disorder. We use a bottom-up growth method to improve edge order. I will present data from both geometries obtained using LEEM, micro-LEED, ARPES, PEEM, micro-ARPES and dark-field PEEM that show the ribbon geometry is very different in the two forms of edge growth. The results complicate simple models for the exceptional transport in these ribbons.

I will also show new ARPES and surface x-ray data that show the buffer graphene layer is in fact semiconducting. SXRD shows that the buffer is not a single layer as usually modeled but is instead a two-layer system of graphene and reconstructed SiC bilayer. Both layer are incommensurate with the bulk. This work offers some insight into why the band gap forms in this buffer graphene layer.

Correlation between Morphology and Transport Properties of Quasi-Free-Standing Monolayer Graphene

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Quasi-free-standing monolayer graphene (QFMLG), obtained by intercalating hydrogen at the interface of buffer layer and SiC(0001), is efficiently decoupled from the substrate and a promising material for wafer-scale graphene-based nanoelectronics [1,2]. However, the mobility of QFMLG is lower than for exfoliated graphene on SiO₂, and the carrier scattering has not been fully understood. Recently it has been reported that the mobility of QFMLG depends on the substrate temperature during the hydrogen intercalation process, and the highest mobility is obtained at 700-800°C [3]. These measurements suggested that the carrier scattering is mainly caused by charged impurities at 600 and 800°C, while defects induce additional scattering at 950°C. We have used scanning tunneling microscopy (STM) to investigate the morphology of QFMLG formed at several hydrogen intercalation temperatures, and discuss its relationship with transport properties [4].

Our STM observations reveal features in the QFMLG formed at 600°C and 800°C which have a diameter of 1.5 nm, a depth of 20-80 pm, and a density of 1×10^{13} cm⁻² (see Fig. 1), and partially align with a periodicity of 1.8 nm, corresponding to the quasi-(6x6) reconstruction of the buffer layer. These features are attributed to incomplete hydrogen intercalation at the graphene-

substrate interface and contribute to carrier scattering as charged impurities. Bilayer-deep voids in the SiC substrate (probably due to etching of the SiC by hydrogen) and wrinkling of graphene appear at 1000°C, and they decrease the carrier mobility significantly.

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Fig. 1: STM image of QFMLG after H intercalation at 800°C. Image size 12 nm × 12 nm.

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"Surface transport below 1 K"

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Research on surface-state superconductivity (or mono-atomic layer superconductivity) has recently been activated by a series of discoveries. It was initiated by *in-situ* transport measurements in UHV at Henzler's group, showing that the superconducting critical temperature $T_{\rm C}$ of a 4 monolayer (ML) thick Pb film on Si(111) substrate was almost the same as that of bulk Pb [1]. It was followed by scanning tunneling spectroscopy (STS) measurements by Shih's group indicating that 2 ML Pb films had $T_{\rm C}$ =4-5 K, significantly lower than the bulk value [2]. And finally STS measurements by Xue's group about nearly one ML Pb on Si(111), showing a surface superstructure (Striped InCommensurate phase), exhibited superconductivity with $T_{\rm C}$ =1.1 K [4]. The technique and apparatus for *in situ* surface transport measurements in UHV are now available even below 1 K under strong magnetic field [5]. An 2 ML-Indium-induced surface superstructure Si(111)-sqrt(7) x sqrt(3)-In [3,4,6,7] and 2 ML Ga on GaN(0001) substrate [8] are also found to be superconducting.

Superconductivity at surface states have multiple viewpoints of interests, two-dimensionality, effect of phonons at surface/interface of the substrate, and lifted spin-degeneracy by Rashba effect. It is recently found that Si(111)-sqrt(3) x sqrt(3) surface, which is composed of 1 ML TI and 1/3 ML Pb on Si(111), exhibits giant Rash splitting in the spin structure of surface states and also superconducting transition around 2.2 K [9]. This can be a parity-broken superconductor with a mixture of singlet and triplet Cooper pairs due to the spin-split surface state band. The surface-state superconductivity is now an emerging topic in surface physics.

A part of the present results is based on the collaboration with Prof. A. A. Saranin's group at Vladivostok in Russia.

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Electron Diffraction at Surfaces: by now Ultrafast!

Michael Horn-von-Hoegen Fakultät für Physik, Universität Duisburg-Essen,

The ultrafast structural dynamics at surfaces can be studied by electron diffraction using a combination of a pulsed electron gun with a fs laser system in a pump probe scheme under ultrahigh vacuum conditions. The grazing incidence of electrons of 30 keV in reflection high energy electron diffraction (RHEED) geometry ensures high surface sensitivity. The sample is excited with 800 nm photons with pulses of 80 fs length, an energy of 1 mJ at 5 kHz repetition rate and a fluence of 1 - 8 mJ/cm² [1-3]. Applying a tilted pulse front scheme for the laser pulses the temporal resolution of the entire setup has recently been improved to less than 400 femtoseconds [4]!

The huge potential of this technique is demonstrated with the non-equilibrium dynamics of the In induced (8x2) reconstruction on Si(111). This surface exhibits a Peierls-like phase transition at 130 K from a (8x2) ground state, which is accompanied by the formation of a charge density wave (CDW), to a (4x1) excited state. Upon excitation by the fs-laser pulse the (8x2) groundstate is driven into the excited (4x1) state at a sample temperature of 30 K. The surface is only excited electronically, the structural transition occurs in 350 fs, but the surface remains for almost one nanosecond in a super-cooled excited (4x1) state. An activation barrier of ~40 meV for the collective motion of the In atoms hinders the immediate recovery of the (8x2) groundstate. Such metastable situation – a hidden state of matter far away from equilibrium – is only accessible through the ultra-fast excitation by the fs-laser pulse. The relaxation to the (8x2) ground state is delayed on a timescale of ~ 500 picoseconds and is triggered by (8x2) remnants pinned at adsorbates that act as nucleation seeds – the same way that super-cooled water in a bottle freezes upon the insertion of seeds. The surface unit cells fall back into their ground state, one at a time, like a row of falling dominoes [5]. From a transient spot profile analysis of the width of the (8x2) spots we can determine the speed of the phase front which propagates at about 100 m/s.

The initial structural transition at a time scale of 350 fs is explained by an accelerated displacive transition and followed by a heating of the surface atoms on a time scale of 3.5 ps. The thermal motion of the indium and silicon atoms is observed by means of the Debye-Waller effect which causes a reduction of intensity of the diffraction spots. On a time scale of 20 ps this thermal motion has dissipated into the Si substrate as evident from the recovery of the intensity.

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Challenges and Prospects of Surface Crystallography by LEED

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In surfaces of complex compound solids and two-dimensional supramolecular structures of organic molecules chemical bonds are formed at different levels, from covalent to Van der Waals. Their interplay determines both the surface geometry and the electronic structure of these surfaces and, hence, detailed structural characterisation can reveal important information about the balance of the interactions involved. Many organic layers have been well characterized at the molecular level, mostly using scanning probe microscopy and/or spectroscopic methods, but experimental crystallographic information at the atomic level is rare; this includes bond lengths and orientations of molecules (intra-molecular, inter-molecular and molecule-substrate) as well as substrate reconstructions in response to adsorption. LEED-IV structural analysis, despite being one of the most powerful techniques for surface crystallography in general, is still facing a number of problems, when applied to organic layers and/or other complex surface structures. Current limitations are imposed by the available computer power for large unit cells but also by the size and quality of the experimental data set and by approximations made in standard LEED-IV codes. We will discuss strategies for improving the data set and modifications to the standard analysis methods that are necessary to make full use of these improvements. The second part of the talk will concentrate on examples of organic layers and nano-structures inorganic surfaces, whose surface crystallography has been determined by LEED, and discuss the implications in terms of chemical bond formation and molecular recognition at surfaces.

Low-energy electron microscopy and micro-diffraction analysis of nanoscale transient cerium oxide phases during reduction by molecular hydrogen

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Ceria is a highly versatile oxide and used in many catalytic applications today; however, its structure-function relation and true active nature in chemical redox reactions are still not well understood. An important example is the interaction of ceria with molecular hydrogen, which is an integral part of the hydrogenation process that produces methanol from CO₂ (CO₂ + 3H₂ \rightarrow CH₃OH + H₂O). Here, employing a powerful combination of electron spectromicroscopy with synchrotron radiation, low-energy electron microscopy, and micro-illumination diffraction analysis, we follow *in situ* the complex structural transformations of a well-defined ceria/Ru(0001) model catalyst system when exposed to a reactive H₂ environment. Specifically, by modeling the time-dependent, experimental diffraction profiles acquired during the reduction process (see left figure) we demonstrate that the transition from CeO₂ to crystalline Ce₂O₃ occurs through a mixture of transient, ordered cerium oxide phases whose average size is on the order of just a few nanometers. Furthermore, these crystalline surface phases are shown to exhibit characteristic intensity-voltage curves, which allow their spatial distribution directly to be imaged in real space (right figure).





Figure: (left) Evolution of the *in situ* LEED profiles (top panel) from a (1x1)-ordered pattern characteristic of fluorite $CeO_2(111)$ to a (4x4) bixbyite $Ce_2O_3(111)$ phase and comparison to simulated diffraction profiles (lower panel). (right) LEEM image of a reduced cerium oxide island with oxidation state contrast.

Crystallographic analysis of one-dimensional metal and metal-oxide hybrid structures formed on the Ir(100) surface

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One third monolayer of cobalt deposited on the unreconstructed Ir(100) surface forms pseudomorphic islands stable up to annealing temperatures beyond 500°C. Oxygen dosage at elevated temperatures (250°C), however, transforms this phase into a homogeneous 3×1 -periodic arrangement of CoO₂ chains. These chains consist of a centre Co wire, which is from a geometrical point of view completely decoupled from the substrate and linked only via the oxygen atoms at both sides. These one-dimensional metal-oxide hybrid structures can be further oxidized by NO₂ decomposition (and NO desorption) forming CoO₃ chains. When the Co wires are fully oxidized by this process, additional oxygen is found to assume fourfold iridium hollow sites in between the CoO₃ stripes. On the other hand, the CoO_x phases can be reduced e.g. by hydrogen at rather low temperatures (80°C) leading eventually to a 3×1 -ordered surface alloy, whereby mono-atomic Co wires are embedded in the outermost Ir layer.

So far, similar metallic and metal-oxide hybrid structures could be prepared only at step edges of vicinal single crystal surfaces (e.g. [2,3]), typically with low density and a poor degree of order. Here, in contrast, these one-dimensional structures grow at maximum density right on the plain terraces of the substrate. Furthermore, the structures grow in a self-organised way with a close to perfect lateral order and so allow for a quantitative characterization by surface diffraction methods.

All the observed phases were crystallographically determined by means of full-dynamical LEED analyses using the Erlangen Tensor-LEED code [3]. For each phase a huge intensity data basis (between 10,000 eV and 20,000 eV) was collected for normal incidence of the primary electron beam and energies ranging up to 800 eV. The final fit structures always yield a very satisfactory agreement between experimental and calculated spectra expressed by Pendry R-factors between 0.090 and 0.116. The low R-factors in combination with the large data bases leads to a positional *precision* of the analyses in the single picometer range, whereby the high energy intensity data are proven to be similarly sensitive to surface atom coordinates as the lower energy data. Furthermore, the *accuracy* of the structural results is impressively demonstrated by a very close correspondence (also in the picometer range) of structural parameters derived from LEED to those originating from DFT total-energy calculations of the respective model structures.

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SPA-LEED and high resolution optical spectroscopy of molecules on surfaces

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SPA-LEED is commonly used to quantify structural correlations of atoms or molecules in the context of growth phenomena or phase transitions at surfaces. However, SPA-LEED can also be most helpful when delocalized excitations in ordered aggregates on surfaces are probed. We report on such an experiment from the field of optical phenomena in ordered molecular aggregates

Surfaces provide a tool to prepare two-dimensional ordered molecular aggregates with structures that are otherwise not realized in the corresponding three-dimensional aggregates. We consider PTCDA on thin epitaxial KCl(100) films. Interestingly, on KCl(100), the PTCDA molecules are all aligned with their long axes, forming a commensurate brickwall (BW) structure, which differs strongly from the herringbone arrangement in bulk crystals. This structure enables a strong coupling between the excited states. The domain sizes, as deduced from the SPA-LEED profiles, can reach several hundred angstroms on well prepared KCl films. The optical spectra show a strong enhancement of the transition as it is expected from the intermolecular coupling of the molecules. However, the line profiles, are still considerably broader than those of isolated molecules.



Comparison of fluorescence exci-tation (FLE) spectra for different phases of PTCDA on the KCl(100) surface. Black: Condensed long range ordered brick-wall (BW) phase (1 ML), red: phase of diluted immobile molecules (d phase, 0.01 ML) at terrace sites, and blue: as before, but molecules at step sites. All spectra have been aligned and normalized at the position of the 0-0 transition of the BW phase (19600 cm⁻¹). The black spectrum is broadened by effects, related to the final size of the PTCDA domains; the red and blue spectra broadened by are inhomogenous distributions of adsorption sites. For the step site this distribution is narrower leading to narrower lines.

To our current understanding [1], this line broadening is related to the finite size of the ordered aggregates on the surface. In order to test this we optimized the size of the domains. We will report on the effect on the optical spectra in correlation with information deduced from SPA-LEED.

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Facet analysis using Atomic Force Microscopy

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Surface sensitive diffraction techniques including SPA-LEED are well-known to yield integral information on surface faceting [1]. In order to obtain information on the spatial arrangement of the facets on the nanometer scale, direct imaging techniques like low-energy electron microscopy are very useful [2]. Scanning probe techniques, in particular atomic-force microscopy (AFM) allow also access to integral information on faceting via the analysis of the histogram of local surface normals derived from AFM images [3,4]. Of course, AFM yields also access to size and shape of the nanofacets [5], even in the case of free-standing nanorods [6].

Here, we apply AFM based facet analysis to chromium poisoned, degraded $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ solid oxide fuel cell samples. As is demonstrated in Fig. 1, the determination of the three-dimensional shape including interplanar facet angles can yield information on the structure and composition of the crystallites evolving during degradation. A good agreement with theoretical angles obtained from crystal structure data for SrCrO₄ (monazite-type) was found.



Figure 1: a) AFM image of an individual crystallite observed on the Cr poisoned, degraded $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ electrode surface. For the four marked facets, the interplanar angles were measured. b) Assuming monazite crystal structure allowed to identify these four facets (orange).

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Au/Ge(001): a wetting-dewetting transition

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The structure and electronic properties of the Au induced nanowire reconstruction on Ge(001) have been under debate [1-14], since their existing was were first reported 10 years ago [1-2]. We have used LEEM and STM to investigate their formation dynamics. At low temperature, the growth of the nanowire domains is limited by diffusion of Au. A wetting-dewetting transition



Fig. 1. An STM image (-1.3 V, 0.8 nA) of a Au cluster imaged at room temperature.

occurs at ~ 665 K that transforms nanowire domains into three-dimensional Au clusters. Dewetting occurs above ~665 K and is fully reversible during repetitive heating and cooling cycles. The decay and growth rates of the nanowire domains below ~665 K show intriguing dynamics, casued by the complex diffusion of gold. It correlates directly with the diffracted intensity of a reconstruction along the top of the nanowires, indicating a temperature-dependent potential landscape for the thermally activated diffusion of Au atoms across nanowire domains.

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Ceremonial talk

Surface Science: Historical Remarks and Martin Henzler's Role

Hans Lüth Forschungszentrum Jülich

The early period of semiconductor surface physics starting after the 2nd world war at Bell Labs in the USA with the aim of developing a solid state amplifier is shortly described. A deeper understanding was achieved by Bardeen's postulate about the existence of surface states. Also the development of LEED by Farnsworth at Brown University for the assessment of clean surfaces is mentioned. In this context the early work of Martin Henzler in the Aachen group on UHV prepared Si surfaces and his development of SPA-LEED in later time shows parallel lines of development. The concept of surface states being important at the beginning of surface science remains exciting even up to these days. This is shortly demonstrated by the unusual properties of the recently detected topologically protected surface states on topological insulator surfaces.

Poster session

(Thursday 16:00-19:00)

LNQE

Please hang up the posters during the first coffee break.

1	Epitaxial growth of thin films of LiCl, KCl and NaCl on the Ag(100) surface C. Brülke, C.Marquardt, A. Paulheim, M. Sokolowski
2	Growth, Structure, and Stability of the High-Index TbO _x (112) Surface on Cu(111) J. Höcker, W. Cartas, A. Schaefer, J. F. Weaver, J. Falta, J. I. Flege
3	Formation and structural observation of ultra-thin high-k silicate films on Si(001) S. Islam, K.R. Hofmann, H.Pfnür
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Epitaxial growth of thin films of LiCl, KCl and NaCl on the Ag(100) surface

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Thin films of alkali halides on metal surfaces are model systems for insulating materials and can be examined by electron spectroscopies without charging effects. We recently analyzed thin films of KCl(100) and NaCl(100) on the Ag(100) surface by spot profile analysis low energy electron diffraction (SPA-LEED) [1,2]. KCl shows epitaxial growth and no rotational mosaicity. The films grow to a domain size of up to 400 Å. NaCl films, on the other hand, show significant rotational mosaicity. The majority of the NaCl domains are in or close to alignment with the unit cell vectors of the Ag(100) surface, but also domains rotated by 45° with respect to the Ag(100) unit cell have been observed. The domains grow to a lateral size of 500 Å.

LiCl on Ag(100) has been examined as a third system in this series. At a growth temperature of 400 K a Volmer-Weber growth mode was found. The SPA-LEED patterns show strong rotational mosaicity with periodic maxima separated by 15° in azimuthal orientation. Four differently oriented types of LiCl domains have grown on the surface. The domain sizes are in a range of 40 - 150 Å. The domains which are rotated by 30° with respect to the Ag[100] direction are the smallest and the domains which are in alignment with the Ag[100] direction are the largest. However, the azimuthal broadening of the spots indicates that there are also LiCl domains in any other orientation with respect to the Ag surface. Supported by the DFG

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Left: 2D LEED pattern of 32 ML LiCl at 91,5 eV and 290 K. LiCl was deposited at 320 KL and annealed at 400 K for 30 min. *Right:* 1D circular scan of the LiCl(10) spots (inner circle in 2D pattern).

Growth, Structure, and Stability of the High-Index TbO_x(112) Surface on Cu(111)

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High-index surfaces of rare-earth oxides, typically found as side facets of rare-earth oxide nanoparticles, are suspected to exhibit a superior catalytic activity in a number of catalytic Due to the lack of model systems, the validity of this hypothesis has not been reactions. experimentally investigated in detail yet. We used low-energy electron microscopy and microillumination low-energy electron diffraction (µLEED) to investigate the structural and morphological properties of terbium oxide films grown on Cu(111) in ultrahigh vacuum. Roomtemperature deposition of terbia on the Cu(111) surface in oxygen background leads to a uniformly covered surface but the grown terbia film lacks long-range ordering. Annealing of this terbia film in oxygen background leads to dewetting of the Cu(111) substrate and a three dimensional, dendritic growth of terbia islands which exhibit a hexagonal (1.4 x 1.4) structure with respect to the Cu(111) surface. In contrast to room temperature deposition we find a Volmer-Weber growth mode of terbia(112) islands on the Cu(111) surface for terbia deposition at elevated temperature which can be identified by nano-illuminated low-energy electron diffraction as well as from a typical rectangular shape of the terbia(112) islands. We also establish the coexistence of (112) and (111) orientated islands surrounded by different copper surface oxides (Fig. 1). Annealing of the coexisting (112) and (111) islands reveals that the TbO (112) phase is less stable



Fig. 1: (a) LEEM image of the surface after terbia deposition at 475°C. (b) TbOx(111) μ LEED pattern recorded from a round-shaped island. (c) TbOx(112) μ LEED pattern obtained from a rectangular-shaped island.

than the (111) phase and decays in favor of the TbO (111) domains.

Formation and structural observation of ultra-thin high-k silicate films on Si(001)

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Formation of barium silicate Ba_2SiO_4 on the Si(001) surface can be amorphous or crystalline, based on growth conditions and applied temperature. We formed both crystalline and semicrystalline silicate and characterized it with SPA-LEED, EDXS, XPS, SIMS, STEM, HRTEM. This silicate was then used as a high-k dielectric in a MOS diode.

Tetragonal crystalline Ba₂SiO₄ was grown at 605°C by evaporation of Ba in oxygen atmosphere after careful adjustment of Ba flux and oxygen pressure. The preferential orientation of silicate crystals is with the 'c' axis perpendicular to the film, as seen by SPA-LEED measurements. In the surface plane two domains form with axes along [110]. In agreement with SPA-LEED, we found with TEM nanocrystallites with in-plane sizes between 10nm and 15nm. The lattice constants of the silicate were measured with SPA-LEED to be a \approx 5.77Å and b \approx 7.61Å, which were also found with TEM, together with c-periodicity of 10.8 Å. Due to silicon diffusion from the substrate, necessary for silicate formation, the interface is rough, which also leads to growth of minority crystals with different orientations. The rough interface seems to be the main reason for the still relatively high interface trap density (10¹² eV⁻¹ cm⁻²), determined in frequency dependent electrical measurements. The lack of any significant hysteresis in capacitance versus voltage (C-V) curves is indicative for a very small concentration of rechargeable bulk defects in the silicate, even though the thicker (>5nm) silicate consists of a mixture of crystalline material at the interface and an amorphous layer on top, as observed in TEM. Crystalline orientation of silicate on Si(001) surface and other properties will be discussed.

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Poster No. 4

Archimedean snub square tiling in a BaTiO₃-derived epitaxial film on Pt(111)

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Under specific preparation conditions, ultrathin $BaTiO_3$ films on Pt(111) develop a 2D quasicrystalline structure of twelve-fold rotational symmetry. This structure is composed by an aperiodic arrangement of triangular, quadratic and rhombic tiling elements [1]. Searching for the basic mechanisms of its formation, a periodic approximant has been identified. It merely consists of the triangular and quadratic elements of the quasicrystal that arrange in a snub square tessellation (Fig. 1a). In vertex notation, this structure can be described as (3.3.4.3.4) pattern, which has already been considered by Kepler in his general analysis of Archimedean tilings [2]. Applying STM, LEED, and SPA-LEED, the corresponding lattice parameters and the epitaxy matrix with respect to the Pt(111) substrate are determined with high precision (Fig. 1b). STS indicates that Ti^{3+} -O- vacancy clusters are constituents of that structure similar to the case which has been deduced for the quasicrystal. The film structure found is an important additional nanoscale observation of the - hitherto rare - five-vertex motives in 2D interface tessellations.

(a) High-resolution STM image of the (3.3.4.3.4) pattern after drift compensation. The characteristic star-configuration of the atomic reconstruction (yellow, green) together with the periodic unit cell (blue) are marked; (U=1.0 V, I=0.3 nA, 4x4 nm², Δz =80 pm). (b) Detail of a SPA-LEED image at 110 eV with BaTiO₃(111)-(1x1) spots (yellow), spots of the quasicrystalline structure (orange) and of the (3.3.4.3.4) pattern (red).

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In-situ growth study of the inverse model catalyst CeO2 /Au(111)

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Cerium oxide (ceria) is well-known for turning the usually inert Au(111) surface into a highly active water-gas shift catalyst [1]. However, little is known about the fundamental growth and interaction mechanisms. In this contribution, a comparative LEEM-based growth study of the inverse model catalyst CeO2 on Au(111) is presented. For this purpose, on the one hand ceria was grown by reactive molecular beam epitaxy (rMBE) and on the other hand by post-oxidation of MBE deposited metallic cerium.

Using rMBE growth in the temperature range between 600°C and 800°C, ceria exhibits a Volmer-Weber like growth mode and forms randomly shaped islands of a few ten to a few hundred nanometers in size (Fig. 1a). LEED and I(V)-LEEM analysis show the cerium oxide to be almost fully oxidized. Depending on deposition temperature, the islands vary in size and nucleation density, with a high density of small islands at lower temperatures, and decreasing density but increasing size at higher temperatures. LEED reveals a preferential collinear azimuthal alignment of the ceria lattice with the substrate, denoted as CeOx A (Fig. 1b). However, there is also a significant amount of off-axis rotational domains (CeOx B), suggesting an overall weaker interaction of ceria with Au in comparison to the well-ordered model system ceria on Ru(0001) [2].



Fig. 1: *a***)** LEEM image of cerium oxide islands grown by reactive MBE at 650°C. *b***)** LEED image of sample shown in a). Cerium oxide reflections are marked by the yellow circle, *c***)** LEEM image of triangularly shaped cerium oxide islands grown by Ce metal deposition and post-oxidation at 650°C.

Post-oxidation of few monolayer thin 2-D films at comparable temperatures to rMBE also leads to the formation of almost fully oxidized cerium oxide islands. Oxidation at coverages of less than one monolayer of Ce metal produces regularly shaped, triangular islands

(Fig. 1c), while randomly shaped islands emerge for oxidation at higher coverages, similar to the case of rMBE growth.

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Crystallographic analysis of oxygen adsorption phases on Ir(100)-1×1

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The adsorption of oxygen on the unreconstructed Ir(100) surface has been controversially discussed in the past. While theoretical studies [1-3] claim different stable adsorption structures over the whole coverage regime, from experimental side only one ordered structure, namely a 2×1-O phase, is reported in literature [3-5]. Besides, also the structure of the 2×1-O phase is not completely clear. While a LEED intensity analysis of this phase by Johnson *et al.* [4] revealed exclusively bridge site adsorption and an oxygen coverage $\theta = 0.5$ ML, a more recent XRD study by Sander *et al.* [3] claimed additional randomly populated hollow sites between the oxygen rows, leading to a total coverage of about 0.65 ML. This situation triggered us to reinvestigate not only the 2×1-O phase but also the whole adsorption system by means of LEED, STM and TDS. Thereby we also entered the experimentally so far unexplored coverage regime $\theta > 0.5$ ML by the application of atomic oxygen sources. In total, we found as much as four ordered oxygen phases on the unreconstructed Ir(100) surface: 3×1-O, 2×1-O, 2×2-3O and 1×1-O phases for nominal coverages of $\theta = 0.33$, 0.50, 0.75 and 1.0 ML.

To reveal the crystallographic structure of all the different phases we have performed fulldynamical LEED intensity analyses based on large intensity data sets taken at normal incidence ($\mathbb{E}_{tot} = 4,000 - 10,000 \text{ eV}$). In all cases a very convincing agreement between calculated and experimental data could be achieved expressed by exceptionally low Pendry R-factors (R = 0.077 -0.136). Moreover, in all cases the structural parameters derived from LEED are in very close correspondence (in the range of picometers) with those originating from DFT total-energy calculations performed for the very same structure models. This holds both for the position of the oxygen atoms and the extended local relaxation patterns within the substrate. It turns out that the 3×1-0, 2×1-0 and 1×1-0 phases show exclusively bridge site adsorption, while the 2×2-30 phase indeed exhibits a mixture of bridge and hollow sites, as predicted by Sander *et al.* [3]. With this new structures the phase diagram of oxygen on the Ir(100) surface turns out to be more complex as previously assumed. The reason that the additional phases remained undetected so far, might be due to the fact that the 3×1 and 2×2 phases exhibit reversible order-disorder transitions at temperatures well below room temperature.

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Oxidation of epitaxial iron films on Ag(001)

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Iron and iron oxides are of great interest in various fields of application due to their large variety of physical and chemical properties. Especially spin-dependent material properties are the reason for phenomena as giant magneto resistance (GMR) and tunneling magneto resistance (TMR). For instance, ferrimagnetic magnetite Fe_3O_4 with (cubic) inverse spinell structure is a promising candidate for such magnetic devices due to its complete spin polarization at the Fermi level. In order to develop these devices and to select certain iron oxide phases it is important to understand the structure and growth properties of such oxide films.

Hence, this work investigates the growth of iron films and, especially, the process of iron oxidation with respect to different annealing temperatures and oxygen pressures. Therefore, pure iron is deposited on Ag(001) substrates by molecular beam epitaxy (MBE) and the oxidation process of the crystalline iron films is divided into the three consecutive steps of pre-oxidation, UHV-annealing and post oxidation.

Surface structure and morphology are analyzed by spot profile analysis low energy electron diffraction (SPA-LEED), while the chemical composition of the surface is investigated by Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS). Additionally, grazing incidence x-ray diffraction (GIXRD) measurements are performed in order to get information about the bulk structure of the deposited films.

The pre-oxidation, which is performed to suppress Ag-segregation, forms partly Fe_2O_3 and Fe_3O_4 with disordered structures at the surface. The following annealing process in UHV reduces the film to FeO and builds a (2 x 1) superstructure in two domains. By post annealing the films at $p(O_2) = 1 \cdot 10^{-5}$ mbar and T = 400°C the largest amount of crystalline magnetite is achieved and the surface exhibits a ($\mathbb{22} \times \mathbb{22}$) R45° superstructure, which is characteristic for Fe_3O_4 . Even higher temperatures in the post oxidation process reduce the film to FeO and a (3 x 6) superstructure in two domains is formed at the surface.

Domain size distributions of PTCDA and MePTCDI on KCI(100) determined by SPA-LEED and optical spectroscopy

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On the KCl(100) surface the organic dye molecules 3,4,9,10-perylenetetracarboxylicacid dianhydride (PTCDA) and N,N'-dimethyl-3,4,9,10-perylentetracarboxylic diimide (MePTCDI) form monolayers with commensurate ($2\sqrt{2}\times2\sqrt{2}$ R45°) brickwall structures. In these structures the molecules are in a head-to-tail arrangement forming two dimensional J-aggregates with interesting optical properties due to the delocalization of the optical excitation.

Both systems show a pronounced superradiant transition in fluorescence (FL) and FL excitation spectroscopy that correlates with the number of coherently coupled molecules, which is given by the size of the ordered domains on the surface. In addition, we observe that the absorption lines are asymmetrically broadened with respect to the line profiles of isolated molecules. For PTCDA on KCl(100) this broadening has been explained by finite-size effects, i.e., a distribution of PTCDA domains of limited lateral size [1]. From the optical line profile it was deduced that the domains have an average size of 7 × 7 molecules and exhibit a Poissonian size distribution. This result was compatible with spot profile analysis low energy electron diffraction (SPA-LEED) data.

In the present contribution we report on two further going experiments. The first was intended to test whether the noted correlation of the optical line profile and the domains size distribution found for PTCDA is also valid for MePTCDI on KCl(100). Secondly, we recently succeeded to prepare PTCDA layers on KCl(100) with much larger domains (by a factor of ~3). Conclusively, we expected to find a much narrower optical line profile for these. However, so far the profiles did not change drastically, although a significant increase in the superradiant behavior is seen.

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LEED pattern *(left)* and hardsphere model *(right)* of the so-called brickwall *(BW)* phase of PTCDA on an epitaxial KCl(100) film on Ag(100).

Structure and growth of hetero-organic layers on noble metal surfaces

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The first organic layer grown on a metal substrate is crucial for the performance of organic electronic since it determines the growth and structure of the subsequent film and influences the charge transport between the electrode and the active organic layer. We investigated such systems by depositing the molecules copper-II-phthalocyanine (CuPc) and 3,4,9,10-perylentetracarboxylic-acid dianhydride (PTCDA) on Ag(111) and Cu(001) in heteromolecular layers. These two molecules were chosen since they are a typical donor-acceptor system that represents a model system for organic electronics.

Different heteromolecular structures could be identified on both surfaces and LEED was applied to determine their geometric structure. The growth of the heteromolecular layers was studied intensively with the LEEM instrument. The experiments showed that the deposition order of the molecules does not influence the final structure on Ag(111) while it determines the structure on Cu(001). The reason for this is that the stronger interaction of the molecules with copper compared to silver leads to a lower mobility and, thus, the formation of heteromolecular layers is hindered on Cu(001) in certain cases. Nonetheless, heteromolecular structures could be produced by the right deposition order and substrate temperature during the deposition.



Fig: LEED images taken during the deposition of PTCDA on a submonolayer film of CuPc on Cu(001). Part (a) shows the LEED pattern of the initial CuPc layer at a coverage of 0.5 ML. Once the deposition is started, new LEED spots appear (b) which indicates the growth of a heteromolecular structure. They get more intense with increasing PTCDA coverage (c).

Surface crystallography by LEED-IV of large organic adsorbates on Ag

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The atomic coordinates of large aromatic molecules adsorbed on surfaces are of great interest in the context of understanding the details of interaction and chemical bonding between the molecules and the substrate. Normal incidence X-ray standing waves (NIXSW) is considered to be the only technique that can provide this information with sufficient precision. Here we report on an alternative, namely the I(V)-analysis of low energy electron diffraction (LEED-IV) on two model molecules, which have been investigated by NIXSW before. The intention is to gain additional structural information by LEED-IV and to test the potential of LEED-IV for larger molecules.

We present results on PTCDA/Ag(100) and NTCDA/Ag(111) showing an encouraging agreement with those from DFT and NIXSW studies. We derive additional structure information on the internal geometry of the molecules, in particular with regards to vertical distortions of the molecule core, as well as the buckling of the substrate surface.

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Top and side views of the adsorption geometries of PTCDA/Ag(100) (a) and NTCDA/Ag(111) (b) as calculated by LEED-IV. Ag atoms are shown in different shades of blue to indicate the vertical deviation \mathbb{D} d from their position in the relaxed uncovered surface (dashed line, d0); H atoms are shown in white, O_{carb}/O_{anhyd} in red/blue and the chemically different C atoms are marked by different colors. In the side views, d denotes the vertical adsorption height; the vertical scale is enlarged by a factor of 4 and referenced against the Bragg plane (dashed line, d_B). For clarity we show only the molecules within one unit cell of the super structure.

Influence of the central metal atom on phthalocyanine-based heteromolecular monolayers: Comparison of CuPC+PTCDA and SnPC+PTCDA on Ag(111)

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In monolayers consisting of two or more organic molecules, the electronic properties of these molecules, as well as their interaction with the surface can differ significantly from those in the monomolecular phases. Phthalocyanines form a very interesting class of components for these mixed monolayers since their interaction with the substrate, as well as their electronic properties can be tailored by exchanging the central metal atom, a process that does not significantly affect the lateral interaction between these phthalocyanines and other molecules in the monolayer.

We present LEED measurements that reveal that the SnPC+PTCDA mixed monolayer system on Ag(111) displays a variety of phases very similar to those found in the CuPC+PTCDA system on the same substrate. One phase of both systems exhibits exactly the same lateral ordering, the so-called mixed brickwall phase (MBW), and is therefore the ideal model system to study the influence of the central metal atom of the PC. NIXSW, XPS and UPS measurements on this phase show that – although exchanging the central metal ion does not change the lateral ordering – the vertical adsorption geometry of the PTCDA molecule is strongly affected.

Growth and evolution of nickel germanide nanostructures on Ge(001)

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Nickel germanide is a promising material system for low-resistance contact formation to Ge device modules integrated into Si-based integrated circuit technologies. In the present work, the formation processes of nickel germanides on Ge(001) have been investigated by means of low-energy electron microscopy (LEEM) and diffraction (LEED) at elevated temperatures ranging from 450 °C to 590 °C.

We show that square-like and rectangular nickel germanide islands evolve after nickel deposition at 450 °C and 530 °C, respectively (Fig. 1a and b). Comparing the two images, it is obvious that the island density is drastically decreased with temperature. An Arrhenius-like behavior of the island density is found in the analyzed temperature range indicating a diffusion limited island formation mechanism. The LEED images show a (2x1) rconstruction before and after nickel deposition. The observation of nearly identical IV-curves hints at a Volmer-Weber growth mode. Subsequent annealing up to 780 °C does not result in further Ostwald ripening but in a loss of LEEM intensity contrast (Fig. 1c and d) which can be explained in terms of nickel germanide diffusion into the bulk. Additional STM, (S)TEM-EDX and XPS measurements corroborate the results and give further insight into structural, morphological, and compositional aspects of nickel germanide nanostructure formation on Ge(001) [1].



Figure 1: Bright-field LEEM images after Ni deposition at 450 °C (a) and 530 °C (b) at 2 eV. Bright-field LEEM images after Ni deposition at 530 °C (c) and after subsequent annealing to 780 °C (d) at 9.5 eV.

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In situ observation of low temperature growth of Ge on Si(111) via RHEED

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The integration of Ge into existing silicon-based technology is the key approach to new functionality extension of Moore's Law. Ge provides the potential to combine photon based data processing with Si complementary metal oxide semiconductor processing (CMOS). Epitaxial Ge films enable a monolithic integration of optoelectronic devices into silicon-based technology. Ge used as buffer system, is a candidate for III-V integration on Si. Having strong light absorption in near-infrared wavelength range as well as a pseudo-direct band gap behaviour ¹ Ge-based Laser systems or Ge photodetectors can be achieved^{2,3}. The pseudo-direct band gap behaviour is only observed in tensile strained Ge films, which makes precise control of growth parameters and strain engineering necessary.

Growth processes in MBE can be analysed and controlled using reflection high energy electron diffraction (RHEED). RHEED is the most widespread method for in situ analysis of thin film surface structure and provides an opportunity for real time observation of epitaxial growth. The initial stages of Stranski-Krastanov growth mode of Ge on Si(111) were investigated by *Ichikawa and Ino* ⁴ for a wide range of temperatures (from RT on with subsequent heating). *Deelman et al.* added in situ strain relaxation studies of Ge epitaxy on Si(111) for temperatures from 450 °C up to 700 °C^{5,6}.

Here, we investigate Ge epitaxy on Si(111) using RHEED in a growth temperature regime of 200 °C to 400 ° C with growth rates around 1 ML/min. The different stages of Stranski-Krastanov growth mode, i.e. wetting layer formation and subsequent islanding, are identified via spot intensity analysis. With increasing Ge layer thickness strain is accumulated due to the lattice mismatch of 4.2% to Si. At a certain critical thickness the film minimizes its total energy, first via elastic then via plastic relaxation. Elastic relaxation proceeds via island formation whereas plastic relaxation is obtained by introduction of misfit dislocations. RHEED provides in situ access to the degree of strain relaxation. Hence, we obtained information about the low temperature dependence of the critical layer thickness^{5–7}. RHEED patterns give additional information on facet orientation of grown islands which is confirmed using Atomic Force Microscopy and Transmission Electron Microscopy.

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Reactive growth of cobalt germanide islands on Ge(001)

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In today's silicon technology, the integration of germanium structures is one of the most promising routes to improve the performance of semiconductor devices, since Ge has superior physical properties, e.g., larger charge carrier mobilities, and it is compatible with Si processing. One of the challenges for Ge device integration is the fabrication of low-resistance metal/Ge contacts, which are particularly important for high-current applications. As metallization contact materials, Co germanides and Ni germanides have the best perspective.

We have investigated the growth of Co germanide on Ge(001) by Co metal deposition using LEEM, LEED, and XPEEM. Both for room temperature deposition followed by thermal annealing [1] as well as for metal deposition at elevated temperature, we observe the formation of Co germanide three-dimensional islands. Extremely anisotropic, needle-like 3D islands extending in {110} directions coexist with rather compact ones (cf. Fig. 1). The needle-like islands come in two shapes, either with or without a flat top facet. Micro-LEED has been used to determine the facet orientations and the atomic structure of the islands.

XPEEM results obtained in x-ray absorption spectroscopy measurements at the Ge L and Co L absorption edge show that for deposition at room temperature, metallic Co is present on the surface that reacts with the Ge during the thermal annealing step. The germanide forms 3D islands, and no Co nor Co germanide remains between the islands Also from the spectroscopy experiments, different types of islands can be identified, pointing towards different CoGe stoichiometries.





Fig. 1: Cobalt germanide islands on Ge(001) after Co deposition at 650°C. Left: Bright-field LEEM. Right: XPEEM (XAS) from a different surface area at the Co L edge.

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Dysprosium silicide phases on Silicon(111)

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Epitaxial thin films of rare earth silicides are of particular interest because of their possible application as low-resistivity contacts to n-type Si [1]. In addition, the formation of Dy silicide nanowires is in the focus of interest [2]. Therefore the growth of Dy on Si(111) in the monolayer regime has been investigated in-situ by Spot Profile Analysis Low Energy Electron Di ffraction (SPA-LEED) and Auger Electron Spectroscopy (AES).

Dy coverages, ranging from sub-monolayers up to several monolayers, were deposited by Physical Vapor Deposition (PVD) at different substrate temperatures. Using the SPA-LEED technique a phase diagram containing a plethora of reconstructions could be derived, including the ($2 \ 3 \ x \ 2 \ 3$), ($3 \ x \ 3$) and ($1 \ x \ 1$) reconstructions known by literature [1]. These experiments have been complemented by Surface X-Ray Diffraction (SXRD) studies. Furthermore, we found a previously unknown structure which is based on the ($3 \ x \ 3$) structure. The existence of striped phases has been concluded from the splitting of super structure spots and can be described by a ($13 \ 3 \ x \ 3$) super structure.

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Antimony adsorption on Si(112) for selective growth of Ge nanostructures

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The adsorption of group III and group V elements on Si surfaces can be employed to tailor the surface properties and change the growth mode and morphology upon subsequent Ge deposition. Different mechanisms can be employed: surface passivation and kinematic limitation for smooth layer growth [1], as well as self-ordered selective growth of Ge nanostructures by surface chemical patterning or facet array formation [2]. In the present work, we used SPA-LEED to investigate the influence of Sb adsorption on the structure and morphology of the Si(112) substrate and of subsequently deposited Ge. The experiments were carried out by students in the framework of a learning-through-research bachelor course. In agreement with literature [3], the clean Si(112) surface has been found decomposed into (111) and (5 5 12) facets. In previous LEED and STM studies, Cho et al. showed [4] that after Sb adsorption at 300°C, the Si(112) surface predominantly exhibits (111) facets. In the high-temperature regime from 600°C to 750°C investigated here, (111) facets are hardly observed, but other orientations can be identified from reciprocal space maps (RSMs, cf. Fig. 1), most prominently (113) facets. At 750°C, (223) are clearly visible as well. In the whole temperature range, facets have been found to occur in the (1 1 2)-(1 1 -1) plane only, indicating a one-dimensional facet array. After Ge deposition, different facet orientations are found, including facets in the different azimuthal planes. This is explained in terms of threedimensional Ge islands that exhibit side facets in these azimuthal directions, as confirmed by ex-







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Structural and plasmonic investigations in Au-chains grown on Ge(001)

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One dimensional electronic systems show exceptional transport properties such as Peierl's transitions or Tomonaga-Luttinger liquid behavior. The latter has been found in self-assembling Au quantum wires on Ge(001). Their plasmonic excitations are expected to exhibit a dispersion relation different from the well-known characteristics in two or three dimensions because of their strong electronic correlations.

However, to understand the nature of electronic mechanisms the atomistic structure, that is still discussed, has to be understood. Using integrating techniques like SPA-LEED, samples of high quality and, consequently, long range order are required.

Different approaches for the preparation of Ge(001) surfaces are known, the most widespread are chemical etching and sputtering. Having a huge influence on the resulting wire properties the surface quality after both methods is investigated systematically via G(S) and H(S) analysis. Best results were achieved in using chemical etching followed by cycles of Ar sputtering at 800 eV and flash annealing. Furthermore, the analysis is used to estimate the structural properties and order range of the quantum wires. The measurements were carried out by means of spot profile analysis low energy electron diffraction (SPA-LEED). The detailed analysis of diffraction profiles strongly favors the model of the Au-induced giant missing row (GMR) structure rather than the heterodimer model. Systematic variation of the initial Au-coverage has revealed further that approximately 0.25 ML of the deposited Au coverage is incorporated into subsurface positions, in this way stabilizing the adsorbate-induced surface structure [1].

The electronic structure was then investigated via energy electron loss spectroscopy (EELS) combined with a SPA-LEED giving access to plasmonic excitations in the quantum wires at both high energy and momentum resolution. For Au coverages above 0.7 ML plasmonic modes appear in the loss spectra. Their dispersion relation increases almost linearly for $k_{||} > 0.1 \text{ Å}^{-1}$, but deviates significantly from known characteristics of a quasi one-dimensional plasmon [2] for $k_{||} < 0.1 \text{ Å}^{-1}$. A contribution coming from Au clusters seen in SEM can be excluded as the FWHM in the loss spectrum decreases steadily with decreasing $k_{||}$. A dipole excitation can also be ruled out since it would be observable down to zero momentum. It turns out that the data can be described best with the model for plasmons in Luttinger-liquids giving another indication of its existence.

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Kinetics and Dynamics of the $(8 \times 2) \leftrightarrow (4 \times 1)$ Phase Transition in the Indium on Si(111) Atomic Wire system

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The Indium (In) induced (4x1) reconstruction on Silicon(111) is a prototype for an atomic wire type arrangement of metal atoms on a surface. It has attracted much attention because the In wires undergo a reversible Peierls like phase transition at TC = 130 K to a (8×2) reconstructed Charge Density Wave (CDW) ground state. In a high resolution LEED study we observed the existence of a robust hysteresis loop upon slow increase and decrease of the sample temperature at TC. The critical temperatures of the transition are TC+ = 135 K and TC- = 125 K for increasing and decreasing temperatures, respectively. The width of the hysteresis loop of 8.6 K is almost independent on the heating and cooling rate and is thus direct evidence for the existence of an energy barrier between the (8×2) ground state and the (4×1) excited state. It unambiguously answers the question about the nature of the phase transition: it is first order.

In a second experiment the phase transition is probed with ultra-fast time-resolved reflective high electron diffraction. Optical pumping of the CDW (8×2) ground state at a base temperature of 30 K triggers the phase transition electronically to an undercooled metastable (4×1) phase. Utilizing a tilted pulse front scheme together with a new 30 keV electron gun design we improved the temporal resolution to less than less 400 fs. The high transversal coherence length of 40 nm allows to follow both the initial dynamics in the unit-cell and the kinetics of the phase front on the nanoscale. At fluences of 4 mJ/cm2 the CDW ground state is lifted across the entire surface on timescales of less than 400 fs. A transient temperature rise of the In-layer was determined through the intensity of the thermal diffuse background intensity utilizing the Debye-Waller effect. The laser induced heating by less than 40 K takes place on timescales 5 times slower than the metal-to-insulator transition which clearly rules out a simple thermal excitation scenario of the phase transition in this pump-probe experiment.

Plasmonic excitations in Au-induced quantum wires on Si(hhk)

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Si(553) and Si(775) surfaces are strongly stabilized by Au adsorption resulting in chain reconstructions of Au and Si atoms. For low temperatures the chains develop a change in periodicity not because of a Peierl's transition but because of frozen spin-polarization. Therefore, they remain metallic at low temperature. Here we study the 1d metallicity of these systems by investigating the plasmons of the spin-split bands.

The sample quality was controlled with SPA-LEED. The plasmon dispersion was then investigated via a combination of EELS and SPA- LEED setup providing both high energy and momentum resolution. Measurements were carried out at room temperature and at 100 K.

Similar to Au/Si(557) [1], the dispersion for Au/Si(553) and Au/Si(775) is linear and only existent along the wires for $k_{||} > 0.07$ Å⁻¹, a typical signature in 1D systems. Compared to Au/Si(557) the slope is smaller by a factor of about 2 reflecting the lower electron density of around 1 × 10⁷ cm⁻¹.

For pure Au covered surfaces the dispersion stays almost linear for all measured $k_{||}$. Perpendicular to the wires a lower conductivity can be extracted from the shape of the Drude tail for $k_{\perp} > 0$ compared to $k_{||} > 0$. Assisted by electron beam bombardement, parts of the residual gas (CO, H₂) are adsorbed on the surface, most likely at the step edges, continuously moving the dispersion to higher energies, finally saturating at 200 meV (150 meV) for Au/Si(553) (Au/Si(775)) for $k_{||} < 0.05 \text{ Å}^{-1}$. We tentatively explain this by an increase of localization along the terraces. This developing quantum well states are expected for electronically well separated states [2].

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Epitaxial Growth of Ultrathin Lead Films on Silicon (111)

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Epitaxial growth of ultrathin Pb films on Si (111) was studied by means of high resolution electron diffraction (SPA-LEED). The Pb-terminated $\beta(\sqrt{3} \times \sqrt{3})$ reconstruction with 1/3 ML Pb-coverage (1 ML = one Pb atom per Si surface-atom = 7.84 × 10¹⁴ Pb atoms/cm²) was prepared by desorption of a larger amount of Pb at 450 °C and was used as a template layer for deposition. The epitaxial growth mode of lead can be observed at low temperatures of 100 K. LEED-intensity-oscillations reflects layer-by-layer growth mode for coverages larger than 3 ML. In the coverage regime of 1-3 ML the diffracted intensity is strongly reduced indicating roughening of the strained Pb film. Films with 3-5 ML thickness are laterally relaxed by forming a network of misfit dislocations which is observed through satellite spots surrounding all integer order spots in the diffraction pattern. A G(S)-analysis surprisingly still indicates an increased vertical layer distance of 3.05 Å, which relaxes to a bulk-like value of 2.87 Å for films of 6 or more ML thickness. This behavior is corroborated through the LEED intensity-oscillations during deposition, which were measured at different diffraction conditions (i.e. different electron energies). Films deposited on the $\beta(\sqrt{3} \times \sqrt{3})$ -reconstruction are azimuthally disordered, which is derived from the banana-like distorted spots in the diffraction pattern. These films are metastable and break up for temperatures above 220 K.

Probing of In(4x1)/Si(111) interwire coupling by transport measurements

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The In(4x1)/Si(111) reconstruction is used as a prototype for understanding of 1D systems of atomic chains. It shows strong anisotropic transport properties and a temperature driven metal-insulator transition (MIT). Although being intensively studied for more than one decade the effect of defects induced by adsorption (e.g. oxygen) and the inherent change of transition temperature are still under current debate.

A better understanding of the influence of atomic sized imperfections and a correlation with transport measurements can be achieved by a spatial constriction of the electron path. This spatial restriction was performed by using a standard Si approach (optical ex-situ lithographic with reactive ion etching). We are showing a systematic investigation of the effects of confinement performed by means of a 4-tip STM/SEM system (cf. Fig. 1). As expected the sensitivity for the anisotropy ratio is highly affected by a spatial confinement [1].

Moreover, the oxygen adsorption dependent transport studies show not only a reduction of conductivity of σ_{\parallel} along the direction of atomic chains but also a decrease in σ_{\perp} perpendicular to the chains (cf. Fig. 2). This has not been seen before and clearly reveals an effective interwire coupling between the chains which is in agreement with recent DFT calculations [2].

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Fig. 1: Resistance measured on spatial confined (mesa) and unconfined area (2D-infinite) depending on angle of tips aligned in square configuration along In chains.



Fig. 2: Conductivity parallel and perpendicular to the In chains depending on the oxygen dose.

On the microscopic structure of the Ag(441) surface

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Regularly stepped (vicinal) surfaces provide a convenient path to control the number of defects of a surface. They can be easily prepared by a slight miscut of a low index surface. In the case of an fcc(nn1) surface with small integer n it is even expected that the large number of steps will dominate the surface properties.

Here we report on a study of the Ag(441) surface with a combination of scanning tunneling microscopy (STM) and high resolution electron diffraction (SPA-LEED). The STM data suggest a statistical distribution of the step width which can be described in general by a Γ -probability distribution. In fact, the steps are not randomly distributed but are interacting. The detailed statistical analysis of the images also reveals that the terraces are formed by an integer number of (331) building blocks whereas the actual steps are given by (551) microfacets. Complementary to the STM data, reciprocal space maps (RSMs) were recorded using SPA-LEED. In order to compare the electron diffraction data to the real space information from the STM experiment, we carried out simulations of the reciprocal space maps in the framework of the simple kinematic approximation. In this particular case of narrow, interacting steps one has to be cautious to carry out a correct interpretation of the experimental RSM based on the simple analysis of the splitting of the rods and their tilt angle. Especially the latter is strongly influenced by the correct alignment of the SPA-LEED.



Figure: Sketch of the proposed model of a Ag(441) surface given by (331) microfacets and (110) steps (marked in red). Each (110) step with an adjacent (331) microfacet can be seen as a (551) building block.

Recent Advances in High Resolution Real and Reciprocal Space Photoelectron Emission Microscocopy

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Conventional electron spectroscopy methods are limited in providing simultaneous real and reciprocal or k-space information from small areas under laboratory conditions. Therefore, the characterization of materials with only micron scale sample homogeneity requires new instrumentation. Recent improvements in aberration compensated energy-filtered photoelectron emission microscopy (PEEM) can overcome the known limitations in both synchrotron and laboratory environments.

We present first results from real and reciprocal space photoelectron emission microscopy (PEEM) e.g. on Ag (111) showing high k and high energy resolution using a laboratory based He I and II radiation at room temperature and temperatures below 40K. The combination of a recently developed LHe cooled sample stage with an improved aberration compensated energy-filter allows 30 meV energy resolution while a new type of event counting detector improves the signal to noise ratio of the detector.



Figure 1: Photoemission data excited by a laboratory VUV light source (He II) from a Ag(111) surface at room temperature. The photoemission horizon (\pm 90°start angles) corresponds to 6.0 (\pm 0.1) Å-1. The surface state visible in the centre of the image surrounded by six neighboring surface states defines a circle with a diameter of 5.02 Å⁻¹ used to scale this image

Emergence of a stress induced dislocation network during initial growth of Ag-films on Pt(111)

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We have investigated the emergence, growth and relaxation of a stress induced dislocation network during the initial growth of silver films on Pt(111) at 800 K using low energy electron microscopy (LEEM) in microscopy - and diffraction mode, and spot profile analysis low energy electron diffraction (SPA-LEED). We confirmed the formation of a surface confined alloy in the first layer which near completion of the first layer results in a pseudomorphic layer. Further deposition results in reentrant (partial) alloying. Unconventional growth of the second layer with a remarkable transient heterogeneity was observed. Initially, a mixed layer propagates from the ascending step into the terrace. Later a disordered low density bilayer film emerges, which is seen as the expansion of cauliflower shaped branches from the growth front moving out from the steps. The subsequent densification of this film is accompanied by the emergence of a dislocation network which accommodates surface misfit and unveils itself through the appearance of satellites spots near the integer order peaks in the SPA-LEED diffraction patterns.

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Graphene induced faceting of Ir(557)

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With its great application potential due to the unique electronic structure and the mechanical properties, graphene holds promise for future carbon-based device architectures. Lately, a lot of effort has been invested into the growth of graphene on metal surfaces, due to the possibility of separating the graphene from the surface after growth. In some cases the interaction between graphene and the substrate, in conjunction with the elevated sample temperatures, results in a modification of the substrate surface morphology during growth. Here, we investigate the modification of a regularly stepped Ir(557) surface during catalytic growth of graphene at various ethylene pressures and temperatures with low energy electron microscopy. Ir(557) is a vicinal (111) surface with a miscut of 9.45° in [001] direction.We find growth of graphene flakes and nanoribbons, depending on ethylene pressure and sample temperature. The nano-ribbons grow exclusively along the steps. Both, flakes and nano-ribbons, induce a faceting of the surface during growth. An intercalation of oxygen between the graphene and the faceted surface does not affect the already present facets. The orientation of the facets were determined by reciprocal space mapping and (ex-situ) AFM measurements.



Left: μ -LEED image of a graphene covered area on Ir(557). The group of spots (A) resembles the moire-pattern of graphene on an Ir(111) facet. Right: Reciprocal space map of the same area. The (111) facet is inclined by 9.45° relative to the original (557) orientation. The miscut is preserved via formation of (112) facets.

Exceptional ballistic transport in sidewall graphene nanoribbons

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The patterning of graphene into graphene nanoribbons is an essential task for the development of future graphene based electronic devices. For such ribbons with a well-ordered edge geometry the presence of one-dimensional edge states has been predicted. We use a selective graphitization process on the sidewalls of SiC mesa structures to produce graphene nanoribbons with a width of 40 nm. The local electronic properties of the ribbons are investigated by means of a 4-tip scanning tunneling microscope (STM). In combination with a high-resolution scanning electron microscope (SEM), the precise positioning of all four tips on the nanometer range is possible to perform local transport measurements [1]. Additionally, one of the STM tips can be used for scanning tunneling spectroscopy (STS) to gain an insight into the local density of states. The STS reveals two peaks in the local density of states at the edges of the ribbons which can be attributed to the zeroth subbands in the band structure of a ferromagnetic zigzag graphene nanoribbon [2]. Transport experiments carried out on the very same ribbon show a conductance close to e^2/h for a wide temperature range from 30 K up to room temperature and probe spacings between 1 µm and 10 µm. Description within the Landauer formalism is possible assuming ballistic transport dominated by a single channel. Transport in the second zeroth subband is only detectable for probe spacings smaller than 1 μ m due to the short localization length of carriers in this subband. This manifests in the increase of the conductance to 2 e^2/h at probe spacings below 200 nm. As a consequence, it is possible to selectively measure transport in one or two ballistic channels. Remarkably, 4-point probe and 2point probe configurations result in almost identical conductance values as expected for a ballistic conductor measured with fully invasive probes. This invasiveness of the probes can be used to give further evidence for the ballistic nature of transport, simply by introducing one or two additional passive probes in a 2-point probe configuration. Every additional passive probe doubles or triples the observed resistance, a clear indication for single-channel ballistic transport [3].

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Crystallographic and electronic structure of graphene on the pseudomorphic Cu/Ir(111) substrate

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Understanding the nature of the interaction at the graphene/metal interfaces plays a critical role for the correct description of the graphene-based electron- and spin-transport devices. Here, several factors, such as doping level or/and hybridization of the electronic states of graphene and the metal around the Fermi level defines the properties of such interfaces. Starting from p-doped nearly free-standing graphene on Ir(111), its properties are tailored via intercalation of one monolayer of Cu. The crystallographic and electronic structures of the resulting n-doped graphene layer on the lattice mismatched pseudomorphic Cu/Ir(111) substrate was studied by means of Scanning Probe Microscopy (SPM) and Angle Resolved Photoelectron Spectroscopy (ARPES) in combination with state-of-the-art density functional theory calculations.

Transport measurements on epitaxial Bi_{1-x}Sb_x thin films grown on Si(111)

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The alloy $Bi_{1-x}Sb_x$ is a 3D topological insulator for concentrations between x=0.04 and 0.22 [1]. Thus it has topologically protected metallic surface states and an insulating bulk at these concentrations, making it interesting for transport measurements. In this study thin films are used in order to reduce bulk contributions and to provide the possibility of nanostructuring. The films are grown by in-situ co-deposition on Si(111) substrates. The morphology has been controlled by means of low energy electron diffraction.

Temperature dependent transport measurements for temperatures from 12 to 300 K were performed for films of different stoichiometry ranging from x=0.14-0.22 and thicknesses of 10, 20, 40 and 60 BL. Besides variable range hopping and activated bulk transport, metallic surface transport channels have been identified. At 10 BL the surface transport is strongly suppressed in accordance with measurements on Bi_2Se_3 [2].

Furthermore, magnetotransport measurements up to 4 T were performed in order to determine carrier concentrations, mobilities and scattering times. A 30 BL film with a concentration of x=0.18 was found to have carrier concentrations of n=1·10¹³ cm⁻² and p=2·10¹³ cm⁻² with mobilities of μ_n =2.6·10² cm²(Vs)⁻¹ and μ_p =1.9·10² cm²(Vs)⁻¹. The elastic scattering time of Bi_{0.82}Sb_{0.18} is more than one order of magnitude lower than for Bi, possibly due to the alloying-induced disorder, while the inelastic and spin-orbit scattering times are comparable for both systems [3].

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[2] Taskin, A. et al., Physical Review Letters 109, 066803 (2012)

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