

# **Spot Profile Analysis**

## **Low Energy Electron Diffraction**

### **SPA-LEED Workshop Duisburg**

„Die Wolfsburg“  
Mülheim an der Ruhr  
October 27 - 28, 2016



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## **O r g a n i s a t i o n**

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### ***Organisation:***

Michael Horn-von Hoegen

Physics Department  
University of Duisburg-Essen  
47048 Duisburg, Germany  
phone: +(49)-(0)203 / 379 - 1438  
fax: +(49)-(0)203 / 379 - 1555  
horn-von-hoegen@uni-due.de  
<http://www.uni-due.de/ag-hvh>

Frank Meyer zu Heringdorf

Physics Department  
University of Duisburg-Essen  
47048 Duisburg, Germany  
phone: +(49)-(0)203 / 379 - 1465  
fax: +(49)-(0)203 / 379 - 1555  
meyerzh@uni-due.de  
<http://www.uni-due.de/ag-hvh>

Angela Poddig (Secretary)

phone: +(49)-(0)203 / 379 - 1439  
fax: +(49)-(0)203 / 379 - 1555  
angela.poddig@uni-due.de

### ***Location:***

Katholische Akademie „Die Wolfsburg“  
Falkenweg 6  
45478 Mülheim an der Ruhr  
phone: +(49)-(0)208 / 999 19 - 0  
<http://www.die-wolfsburg.de>

10:50 Opening Remarks

11:00 **Development of Ultrafast Low-Energy Electron Diffraction**

Claus Ropers, University of Göttingen

11:40 **Beyond Thermal Equilibrium: Ultrafast Non-Thermal Melting of a Surface CDW in the In/Si(111) Atomic-Wire System**

Tim Frigge, University of Duisburg-Essen

12:00 Lunch

13:00 **Nanoscale Processes and Growth: Recent Advances in Time-Resolved X-ray Scattering**

Stefan Kowarik, University of Berlin

13:40 **Strain Induced Quasi One-Dimensional Rare Earth Silicides Structures on Si(111)**

Frederic Timmer, University of Osnabrück

14:00 **Au-chains Grown on Ge(100): A Detailed SPA-LEED Study**

Timo Lichtenstein, University of Hannover

14:20 Posters and Coffee

15:30 **Adsorption of Sulfur on Si(111): The (4x4) Myth**

Lars Buss, University of Bremen

15:50 **An Oxide Quasicrystal Derived from SrTiO<sub>3</sub>**

Stefan Förster, University of Halle

16:10 **Electronic Fingerprinting of the Conducting Interface During Growth of LaAlO<sub>3</sub> on SrTiO<sub>3</sub> by In-Situ Pulsed Laser Deposition in LEEM**

Alexander J.H. van der Torren, Leiden University

16:45 Conference Outing: Visit to the Gasometer in Oberhausen

19:45 Dinner at Brauhaus Zeche Jacobi, CentrO-Promenade Oberhausen

7:30 Breakfast

8:30 **Metal Growth on and under Graphene: Morphology, Growth Mode and Intercalation**

Michael C. Tringides, Iowa State University Ames Laboratory – USDOE

9:10 **Investigation of Cesium Adatom Superlattice on Epitaxial Graphene**

Marin Petrović, University of Zagreb, University of Duisburg-Essen

9:30 **Quantum Size Effects Induced Stabilization of “Thick” (Near-) Surface Confined Pt-Ge Alloy Films on Ge(001)**

Arie van Houselt, University of Twente

9:50 Posters and Coffee

10:40 **Decay of Isolated Hills and Saddles on Si(001) Studied by LEEM**

Pierre Kirschbaum, University of Duisburg-Essen

11:00 **The Complex Interplay of Thermodynamics and Kinetics in Ruthenium Oxidation**

Jan I. Flege, University of Bremen

11:20 **Resonant Scattering of (very) Low Energy Electrons from the Root-Three BiCu<sub>2</sub>/Cu(111) Surface Alloy**

Bene Poelsema, University of Twente

11:40 **Transport Measurements on Epitaxial Bi<sub>1-x</sub>Sb<sub>x</sub> Thin Films Grown on Si(111)**

Julian Koch, University of Hannover

12:00 Lunch

13:00 **Photoemission Tomography: Imaging the Orbitals of Adsorbed Molecules with Angle Resolved Photoemission**

Michael G. Ramsey, University of Graz

13:40 **Growth of CuPc and NTCD A on Cu(001) Studied by LEED and LEEM**

Christian Kumpf, Jülich Research Center

14:00 **Surface Crystallography of PTCDA on Ag(100) by LEED-IV Using Fourier Coefficients**

Ina Krieger, University of Bonn

14:20 Concluding Remarks

## Development of Ultrafast Low-Energy Electron Diffraction

**Simon Schweda<sup>1</sup>, Gero Storeck<sup>1</sup>, S. Schramm<sup>1</sup>, Max Gulde<sup>1</sup>, Kai Roßnagel<sup>2</sup>,  
Sascha Schäfer<sup>1</sup>, Claus Ropers<sup>1</sup>**

<sup>1</sup>University of Göttingen, Germany;

<sup>2</sup>University of Kiel, Germany

Email: claus.ropers@uni-goettingen.de

“Ultrafast electron diffraction” (UED) comprises a set of powerful experimental tools to obtain detailed insights into rapid structural and electronic processes in solids and gases. In these pump-probe techniques, a short laser pulse induces a structural or electronic change in a sample, which is subsequently probed by diffraction using a short pulse of electrons. In the past, most applications of UED employed electron pulses of high kinetic energies in the range of 10-200 keV, in some cases extending to few MeV, and studied structural dynamics in thin films by diffraction in transmission. In order to gain access to structural dynamics at surfaces, also the grazing incidence geometry of reflection high-energy electron diffraction (RHEED) was successfully equipped with femtosecond temporal resolution. However, for a variety of reasons, the realization of ultrafast low-energy electron diffraction (ULEED) as a structural dynamics tool with ultimate surface sensitivity remains highly desirable. In the past, a host of experimental challenges, including the particularly detrimental effects of electron pulse dispersion at low electron kinetic energies, prevented the implementation of ULEED.

This talk will present first results from our development of ULEED for both transmission and reflection geometries. In particular, we designed and fabricated extremely compact electron gun assemblies carrying laser-triggered nanotip photocathodes, and we use these setups to study different types of structural phase transitions. In a transmission diffraction experiment achieving monolayer sensitivity, we recorded the temporal evolution of the order-to-disorder transition of a polymer/graphene bilayer system following intense optical excitation [1]. Presently, we are conducting the first ULEED experiments in backscattering diffraction [2]. Specifically, we investigate optically-induced transitions between charge density wave (CDW) phases at a single-crystalline 1T-TaS<sub>2</sub> surface. In particular, we observe the transition from the nearly-commensurate (NC) to the incommensurate (IC) CDW phase. By monitoring the temporal change of the IC diffraction spot profiles, we identify a domain coarsening in the nascent IC phase.

Our results demonstrate the potential of ULEED for the investigation of complex, ultrafast structural processes at surfaces. In the future, ULEED will serve as a valuable tool to study the dynamics of surface reconstructions, complex adsorbate superstructures and other quasi-two-dimensional systems exhibiting topologically controlled ordering.

## References

- [1] M. Gulde *et al.*, Science **345**, 200 (2014)
- [2] S. Schweda *et al.*, in preparation (2016)

## Notes

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## **Beyond Thermal Equilibrium: Ultrafast Non-Thermal Melting of a Surface CDW in the In/Si(111) Atomic-Wire System**

**Tim Frigge, Bernd Hafke, Boris Krenzer, Michael Horn-von Hoegen**

Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen,  
Lotharstr. 1, 47057 Duisburg, Germany  
tim.frigge@uni-due.de

The wire-type arrangement of Indium atoms on a Silicon(111) surface serves as a famous prototype for the formation of a (quasi-)one-dimensional charge density wave (CDW) groundstate. At room temperature, the indium atoms are arranged in parallel zig-zag chains, forming a metallic (4x1) structure. Cooling the system down below a critical temperature of  $T_c = 130$  K leads to a structural phase transition: the indium atoms rearrange to hexagons, the periodicity doubles and an (8x2) reconstructed groundstate occurs. The structural transition is accompanied by a metal-to-insulator transition (MIT) through the opening of a bandgap in the electronic structure of about 100 meV.

Ultrafast time-resolved electron diffraction was used to investigate the transient non-equilibrium structural dynamics of the (8x2)  $\rightarrow$  (4x1) phase transition. In this pump-probe setup the sample is excited with 80 fs laser pulses at a peak wavelength of 800 nm and probed with sub-300 fs electron pulses in a surface sensitive geometry, i.e., under reflection at grazing incidence angles of  $1^\circ$  to  $6^\circ$ . Utilizing a tilting pulse front scheme we improved the overall temporal resolution of this setup to less than 350 fs.

Excitation of the (8x2) groundstate with fs-laser pulses revealed the existence of a metastable (4x1) phase. This supercooled phase survives for hundreds of picoseconds due to an energy barrier of 40 meV. However, at fluences of  $7 \text{ mJ/cm}^2$  the CDW groundstate is lifted across the entire surface within 350 fs. A transient temperature rise of the Indium layer was determined through the intensity of the thermal diffuse background utilizing the Debye-Waller effect. The laser induced heating by less than 80 K takes place on timescales 6 times slower than the MIT, which clearly rules out a simple thermal excitation scenario of the phase transition. Instead, we explain the observed dynamics through a displacive excitation scenario, where the optical excitation of the electronic subsystem modifies the potential energy surface of the system. What follows is the accelerated collaborative motion of the surface atoms into the energetically favored (4x1) phase. The phase transition time scales exponentially with the number of excited electrons, i.e. with the laser fluence. Recent DFT calculations (A. Lücke, W.G. Schmidt, Uni Paderborn) confirm this scenario and show that highly specific electronic states have to be occupied to excite the relevant phonon modes which drive the structural transformation within  $1/4^{\text{th}}$  of a soft mode period.



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## **Nanoscale Processes and Growth: Recent Advances in Time-Resolved X-ray Scattering**

**Stefan Kowarik**

Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany  
stefan.kowarik@physik.hu-berlin.de

We present recent advances in time-resolved in-situ X-ray methods for studying growth processes. For the examples of organic semiconductors C60 and PTCDI-C8 we demonstrate how one can measure the 'Henzler'-ring to follow nucleation and lateral structure. Together with X-ray growth oscillations for measuring multilayer growth one gets a fairly complete picture of growth. This in turn makes it possible to use mean-field nucleation theory or kinetic Monte Carlo simulations for predictive simulations and estimates of energy barriers of molecular scale motion. We will finish with an outlook on how a detailed understanding of growth can be used for advanced growth control schemes using fast substrate temperature modulation or light as control parameter

## Notes

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## Strain Induced Quasi One-Dimensional Rare Earth Silicides Structures on Si(111)

**Frederic Timmer<sup>1</sup>, Robert Oelke<sup>1</sup>, Christof Dues<sup>2</sup>, Simone Sanna<sup>2</sup>, Wolfgang Gero Schmidt<sup>2</sup>, Martin Franz<sup>3</sup>, Stephan Appelfeller<sup>3</sup>, Mario Dähne<sup>3</sup>, Joachim Wollschläger<sup>1</sup>**

<sup>1</sup>Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück

<sup>2</sup>Lehrstuhl für theoretische Physik, Universität Paderborn, 33095 Paderborn

<sup>3</sup>Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin

Rare earth (RE) covered silicon surfaces have been in the focus of research for more than 30 years due to their unique properties. For instance, thin RE-silicide films on n-type Si(111) possess very low Schottky-barriers in conjunction with an abrupt surface making them interesting as ohmic contacts. Furthermore RE-silicide nanowires might be applicable as interconnects in future nanodevices or as plasmonic waveguides due to their quasi one-dimensional structure.

Here, we report on a  $(2\sqrt{3}\times\sqrt{3})$  R30° reconstruction for RE coverages exceeding 1 ML which is therefore related to the well-known  $(\sqrt{3}\times\sqrt{3})$  R30° reconstruction. We characterize the structure of the silicide films by means of Low Energy Electron Diffraction (LEED) including Spot Profile Analysis (SPA-LEED), Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) developing a complex model for the reconstructed surface including formation of quasi one-dimensional structures, due to striped domains.

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## Au-chains Grown on Ge(100): A Detailed SPA-LEED Study

**Timo Lichtenstein**<sup>1</sup>, Heiko Teiken<sup>1</sup>, Herbert Pfnür<sup>1</sup>, Joachim Wollschläger<sup>2</sup>,  
Christoph Tegenkamp<sup>1</sup>

<sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover

<sup>2</sup>Fachbereich Physik, Universität Osnabrück

Ge(100) is known as a substrate for self-organized growth of one-dimensional quantum wires by adsorption of Au. Those wires were shown to exhibit spectroscopic signatures of strong electronic correlation. As shown by C. Blumenstein *et al.* (Nature 7, 776) the signatures of this proposed Luttinger liquid behavior depends crucially on the quality of the ensemble and, consequently, on the quality of the Ge(100) sample prior to adsorption. Furthermore, the atomistic structure of these wires is still controversially discussed.

In this study, the morphology has been investigated by means of spot profile analysis low energy electron diffraction (SPA-LEED). We measured systematically the properties on variously prepared surfaces. From G(S)- and H(S)-analyses on ex-situ chemically treated Ge-samples followed by in-situ thermal annealing reveal step heights of 1.42 Å with average terrace lengths around 20 nm and an RMS-roughness of 1.3 Å. Carrying out multiple in-situ Ar<sup>+</sup>-sputtering and high-temperature annealing cycles, the terrace width increases to around 100 nm, the roughness slightly decreases.

After the growth of the Au-wires, the G(S)-curves feature additional structures corresponding to step heights of 1.8 Å which we suggest to be due to the interference of the reshaped gold induced surface structure with the underlying bulk. The detailed analysis of diffraction profiles favors strongly to the model of an 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 penetrates into subsurface positions stabilizing the adsorbate-induced surface structure.

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## Adsorption of Sulfur on Si(111): The (4x4) Myth

**Lars Buss<sup>1</sup>, Thomas Schmidt<sup>1</sup>, Moritz Ewert<sup>1</sup>, Gunnar Schönhoff<sup>2</sup>,  
Tim Wehling<sup>2</sup>, Jens Falta<sup>1</sup>**

<sup>1</sup>Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1,  
28359 Bremen, Germany

<sup>2</sup>Institute of Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1,  
28359 Bremen, Germany

A major task for the integration of novel materials, such as transition metal dichalcogenides, into silicon technology is to adequately functionalize the Si surface. In this context it has been shown that sulfur termination of Si can be used, e.g., for electrical passivation of Si solar cell devices [1], or for subsequent growth of CuInS<sub>2</sub>, a layered material [2]. Interestingly, for the latter the epitaxial quality was found better on S/Si(111) than on S/Si(001) substrates, which has been attributed to a well-ordered S/Si(111) reconstruction (identified as 4x4) by Metzner *et al.* [3], while only disordered surfaces were observed for S/Si(001).

We investigated the adsorption of elemental S deposited from an electrochemical cell on Si(111) as a function of the preparation conditions, using in-situ SPALEED. While an ordered surface phase cannot be produced by room temperature deposition and subsequent annealing, a (4x4) like LEED pattern is obtained for adsorption at elevated temperature. The temperature window for the formation of the (4x4) reconstruction turns out to depend on S flux, indicating that redesorption of sulphur containing species is an important competitive process. This also leads to surface roughening by etching for prolonged deposition, as revealed by G(S) analysis.

From a thorough analysis of the LEED pattern over a wide energy range, systematically cancelled reflections  $\mu$  were identified, implying that the unit mesh is not a hexagonal (4x4) one, but a rectangular  $\begin{pmatrix} 2 & 0 \\ 1 & 2 \end{pmatrix}$  mesh that exists in three rotational domains. This is confirmed by scanning tunneling microscopy.

Based on symmetry arguments inferred from the SPALEED results, two structural models have been proposed and will be presented, one with single S atoms on bridge sites and one with S dimers on bridge sites. Both models have been tested using density-functional theory (DFT). From the DFT-relaxed configurations, the dimer model is preferred. This is in agreement with calibration experiments using x-ray photoelectron spectroscopy, which yield a S surface coverage very close to one monolayer, which is the expected value for the dimer model.

## References

- [1] A. Saha, H. Zhang, W.-C. Sun, and M. Tao, ECS J. Sol. State Sci. Technol. **4**, P186 (2015)
- [2] H. Metzner, Th. Hahn, J. H. Bremer, and J. Conrad, Appl. Phys. Lett. **69**, 1900 (1996)
- [3] H. Metzner, Th. Hahn, and J. H. Bremer, Surf. Sci. **377**, 71 (1997)



## Notes

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## An Oxide Quasicrystal Derived from SrTiO<sub>3</sub>

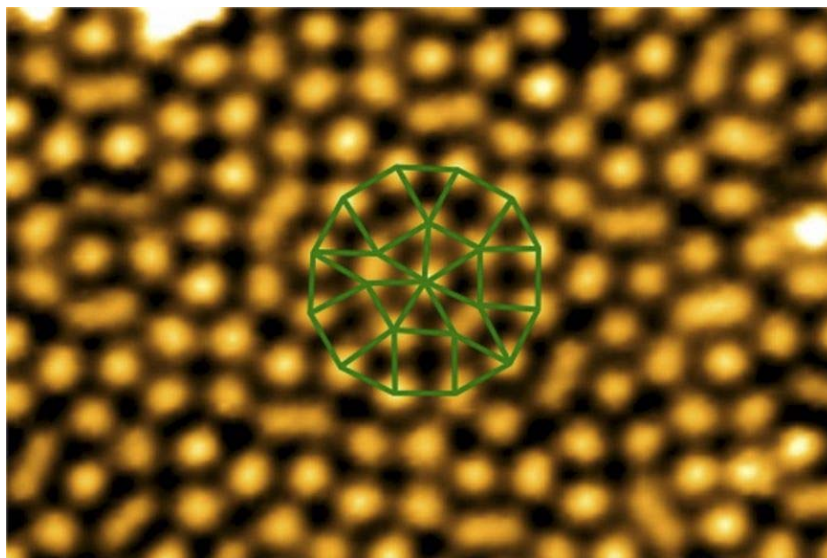
**Stefan Förster<sup>1</sup>, Sebastian Schenk<sup>1</sup>, Rene Hammer<sup>1</sup>, Bettina Leibundgut<sup>1</sup>, Maximilian Paleschke<sup>1</sup>, J. Pantzer<sup>1</sup>, Klaus Meinel<sup>1</sup>, Florian Schumann<sup>1</sup>, Wolf Widdra<sup>1,2</sup>**

<sup>1</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

<sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

In addition to the well-known intermetallic and soft quasicrystals, recently a two-dimensional oxide quasicrystal (OQC) has been discovered [1]. This OQC is derived from BaTiO<sub>3</sub> thin films on a hexagonal Pt(111) substrate. Low-energy electron diffraction (LEED) reveals a twelve-fold rotational symmetry. Scanning tunneling microscopy (STM) at room temperature as well as at low temperatures (80 K) allow to resolve the atomic structure. The aperiodic structure is formed by primitive atomic arrangements in squares, triangles, and rhombs with a universal edge length of 0.69 nm. The resulting tiling is comparable to an ideal Stampfli-Gähler tiling [2].

The observed interface-driven formation of a 2D OQC is not limited to this particular materials combination. Following an analogous preparation procedure, we show that SrTiO<sub>3</sub> on Pt(111) develops an OQC as well. As a consequence of the 2% smaller lattice constant of SrTiO<sub>3</sub> in comparison to BaTiO<sub>3</sub>, the fundamental length of the SrTiO<sub>3</sub>-derived OQC is 2% smaller. Nevertheless, the epitaxial alignment of the SrTiO<sub>3</sub>-derived OQC with respect to the Pt(111) lattice as determined by LEED as well as the local atomic arrangement as measured by STM are identical with that of the BaTiO<sub>3</sub>-derived OQC. Our results suggest that OQC formation is a general process of perovskite oxides on suitable substrates.



**Figure 1:** Atomically resolved LT-STM image of the Stampfli-Gähler tiling of the SrTiO<sub>3</sub> derived OQC. 9x6 nm<sup>2</sup>, I = 5pA, U = 4V.

## References

- [1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature* **502**, 215, (2013)
- [2] F. Gähler in: *Quasicrystalline Materials* (World Scientific, 1988)

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## Notes

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## Electronic Fingerprinting of the Conducting Interface During Growth of LaAlO<sub>3</sub> on SrTiO<sub>3</sub> by In-Situ Pulsed Laser Deposition in LEEM

**Alexander J.H. van der Torren<sup>1</sup>, Zhaoliang Liao<sup>2</sup>, C. Xu<sup>3</sup>, Nicolas Gauquelin<sup>4</sup>, Chunhai Yin<sup>1</sup>, Sense Jan van der Molen<sup>1</sup>, Jan Aarts<sup>1</sup>**

<sup>1</sup>Leiden University, Huygens-Kamerlingh Onnes Laboratorium, Leiden, Netherlands

<sup>2</sup>Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, The Netherlands.

<sup>3</sup>Institut für Solarenergieforschung GmbH Hameln/Emmerthal, Germany

<sup>4</sup>EMAT, Department of Physics, University of Antwerp, Belgium.

Email: torren@physics.leidenuniv.nl

By combining low-energy electron microscopy (LEEM) with pulsed laser deposition (PLD), we have created a unique set-up to study the first stages of growth of complex metal oxides. We demonstrate this by investigating the growth of SrTiO<sub>3</sub> (STO) and LaAlO<sub>3</sub> (LAO) on STO in real-time. For optimal growth conditions and a LAO thickness above the critical thickness of 4 unit cells the interface between these band insulators shows conductivity. We find profound differences in the electronic fingerprint of samples that either do or do not feature a conducting LAO/STO-interface.

In the case of STO on STO, we follow growth by monitoring the intensity and the full-width-half-maximum (FWHM) of the specular diffracted beam at various energies. For layer-by-layer growth, we find the anticipated intensity peaks at the completion of each layer, and an oscillatory FWHM with the maximum at half-layer coverage. Cross sections of the specular beam give more information on the island size while real-space images directly show changes in the shape of step edges and terraces.

For LAO on STO, with the LAO thickness around the critical thickness  $d_{cr}$  of 4 unit cells, the interface becomes conducting. Growing at 780° C in an oxygen pressure of  $5 \times 10^{-5}$  mbar, we observe growth oscillations. Additionally, we measure the intensity of the specular beam as a function of both energy and momentum parallel to the surface. This allows us to extract the band dispersion of unoccupied electron states of the sample surface at regular intervals during growth [2]. Significant differences in the unoccupied band structure develop between samples which are conducting (LAO grown on a TiO<sub>2</sub> termination) and non-conducting (LAO grown on a SrO termination; LAO grown under sub-optimal conditions).

### References

- [1] A. Ohtomo, *et al.*, Nature **427**, 423–426 (2004).
- [2] J. Jobst, *et al.*, Nature Communications **6**, 8926 (2015).

## Notes

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## Metal Growth on and under Graphene: Morphology, Growth Mode and Intercalation

Michael C. Tringides

Department of Physics Iowa State University Ames Laboratory – USDOE  
email: mctringi@iastate.edu

Graphene based electronic and spintronic devices require understanding of the growth of metals on graphene. Several metals (Gd, Dy, Eu, Fe, Pb) deposited on epitaxial graphene were studied with STM, SPA-LEED and DFT. The grown morphology (island density and domain size distributions) was used to extract the metal diffusion and adsorption barriers. For practically all metals the grown mode is 3-d as a result of (i) the low ratio of the metal adsorption to metal cohesive energy and (ii) the repulsive interaction of unscreened charges at the metal-graphene interface that favours islands of small “footprint”. These experimental results are fully supported with DFT calculations [2]. It is essential to find ways to modify the growth to layer-by-layer for high quality metal contacts and for using graphene as a spin filter. By growing Dy at low temperatures or high flux rates it is found that upward adatom transfer is kinetically suppressed and layer-by-layer is possible [3].

Graphene intercalation provides a novel way to tune its properties. Experiments on graphene partially intercalated with Dy show that nucleation is preferred on the intercalated than on the pristine areas. Difference in doping between the two areas generates an electric field that transforms random to directional diffusion and accounts for the guided nucleation [4]. This can be a general method to control patterning of metallic films on graphene.

Many issues related to the intercalation process itself are poorly understood, i.e. the temperature where atoms move below graphene, different intercalation phases, their coverage, the entry points for atoms to move below, the intercalation time etc. SPAL-LEED has been used to study these questions for Dy intercalation in graphene. Spot profiles of several spots (specular, 6sq(3), graphene) are studied as function of temperature and electron energy to deduce the kinetics of intercalation and the layer where atoms reside. This information is essential to tune the emerging properties of intercalated graphene.

In collaboration with D. McDougall, H. Hattab, M.T. Hershberger, M. Hupalo, M. Horn von Hoegen, P. A. Thiel.

### References

- [1] M. Hupalo *et al.*, *Advanc. Mater.* **23**, 2082 (2011)
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- [3] D. McDougall *et al.* *Carbon* **108**, 283 (2016)
- [4] X. Liu *et al.*, *Nano Research* **9**(5), 1434 (2016)

## Notes

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## Investigation of Cesium Adatom Superlattice on Epitaxial Graphene

**Marin Petrović**

Institute of Physics, Bijenička 46, Zagreb 10000, Croatia  
Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen,  
Lotharstr. 1, 47057 Duisburg, Germany

Understanding of graphene's interaction with other atoms and molecules is utterly important due to the potential applications in various devices where graphene is in direct contact with other materials. Frequently exploited systems for studying those interactions are epitaxial graphene samples on various metal substrates where iridium (111) surface stands out due to the preservation of many important intrinsic properties of graphene. However, graphene on Ir(111) also shows clear signs of interaction with the substrate, such as the moiré structure and charge transfer. Those features, among others, provide leverage for further modification and exploitation of graphene.

Here we study adsorption and intercalation of cesium atoms on and underneath the graphene on Ir(111). Angle-resolved photoemission spectroscopy is utilized for determination of the electronic structure while the scanning tunneling microscopy provides an insight into the morphology of the system at the nano-scale. Cesium adsorption on graphene results in electron transfer to graphene, leaving cesium ions positively charged. At high enough concentrations, cesium adatoms form hexagonal domains where the structure within domains is dictated by the Coulomb repulsion between the adatoms and the spatially modulated adsorption energy to graphene which is induced by the moiré structure. In addition, adsorption properties on graphene are explored by depositing cesium atoms on partially intercalated (and therefore inhomogeneously doped) graphene. It is found that the intercalation modifies graphene work function which directly influences the adsorption energy of the adatoms and causes preference of adsorption to non-intercalated graphene areas.



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## **Quantum Size Effects Induced Stabilization of “Thick” (Near-) Surface Confined Pt-Ge Alloy Films on Ge(001)**

**Bene Poelsema<sup>1</sup>, Ali Safaei<sup>1</sup>, Arie van Houselt<sup>1</sup>, Harold J.W. Zandvliet<sup>1</sup>, Raoul van Gastel<sup>1</sup>**

<sup>1</sup>Physics of Interfaces and Nanomaterials, MESA<sup>+</sup> Institute for Nanotechnology,  
University of Twente, P.O.Box 217, 7500AE Enschede, The Netherlands  
Email: a.vanhouselt@utwente.nl

Low Energy Electron Microscopy experiments on the Pt/Ge(001) system demonstrate the formation of a eutectic liquid surface film, after deposition of about 2-3 monolayer-equivalents of Pt and subsequent heating to above about 1003 K. Its composition is consistent with that of the bulk  $\text{Ge}_{0.78}\text{Pt}_{0.22}$  eutectic. Triggered by the eutectic, a near surface confined  $\text{Ge}_3\text{Pt}$  compound emerges upon cooling below  $T_C$ , which has an abrupt interface with the Ge(001) substrate and which is absent in the Ge-Pt bulk phase diagram. From Fabry-Pérot type oscillations in the LEEM intensity versus energy curves we conclude that the  $\text{Ge}_3\text{Pt}$  film contains coexistent regions with thicknesses of about 5 and 9 layers, corresponding to 0.70 and 1.26 nm, respectively. The unanticipated  $\text{Ge}_3\text{Pt}$  phase is attributed to Quantum Size Effects (QSE): the robustness of these films is enhanced by standing wave patterns of Fermi electrons between the surface and the abrupt hidden interface. We conclude that QSE stabilization of the surface phase prevents the redistribution of Pt into a highly diluted state in bulk Ge and suggest that this phenomenon may well be more general.

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## Decay of Isolated Hills and Saddles on Si(001) Studied by LEEM

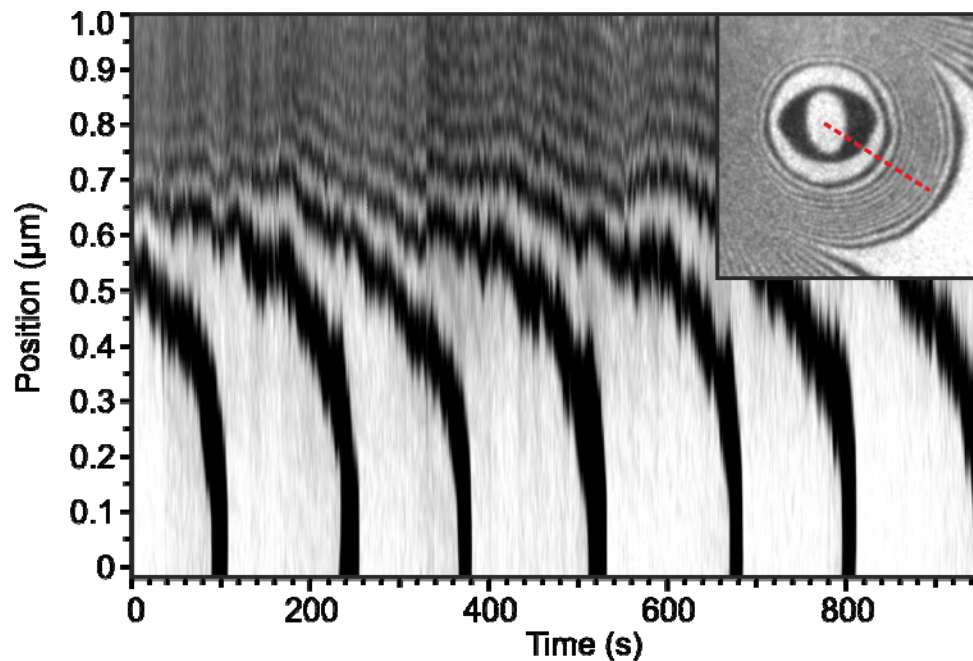
Pierre Kirschbaum<sup>1</sup>, Lothar Brendel<sup>1</sup>, Kelly R. Roos<sup>2</sup>, Michael Horn-von Hoegen<sup>1</sup>, Frank-J. Meyer zu Heringdorf<sup>1</sup>

<sup>1</sup>Faculty of Physics and Center of Nanointegration Duisburg-Essen (CeNIDE),  
University of Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

<sup>2</sup>Present Address: Faculty of Engineering and Physics, Bradley University, Preoria, IL 61625

Dark field low energy electron microscopy is used to study the high temperature decay of isolated hills and saddle points on Si(001). We find different temperature dependent decay rates for the top of the hill compared to a saddle point with low step density that is present in the vicinity of the hill. Due to the Gibbs-Thomson effect, the decay rate of the hill is always higher than the decay rate at the saddle. The two rates converge with increasing temperature and become equal at temperatures above 1060°C. We also report an alternating fast and slow decay rate for the layer-by-layer decay of the hills. This surprising finding is independent of temperature and is caused by a broken symmetry due to a macroscopic strain in the sample.

Furthermore, *in-situ* deposition of gold on the Si(001) surface increases the decay rates of the hill and saddle by more than a factor of ten. This effect can be explained by a formation of a kind of surface-eutectic which reduce the melting point locally.



**Figure 1:** Cross section through a decaying hill as function of time at a surface temperature of about 920°C. The time constant of the decay, as well as the decay rate are larger for every second top terrace of the hill.

## Notes

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## The Complex Interplay of Thermodynamics and Kinetics in Ruthenium Oxidation

**Jan I. Flege<sup>1,2</sup>, Benjamin Herd<sup>3</sup>, Jan Lachnitt<sup>4</sup>, Martin Hoppe<sup>1</sup>, Jan Höcker<sup>1</sup>, Jan C. Goritzka<sup>3</sup>, Herbert Over<sup>3</sup>, Eugene E. Krasovskii<sup>5</sup>, Jens Falta<sup>1,2</sup>**

<sup>1</sup>Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

<sup>2</sup>MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany

<sup>3</sup>Department of Physical Chemistry, Justus-Liebig-University, Heinrich-Buff-Ring 58, 35392 Gießen, Germany

<sup>4</sup>Faculty of Mathematics and Physics, Department of Surface and Plasma Science, Charles University in Prague, V Holešovičkách 2, 18000 Prague 8, Czech Republic

<sup>5</sup>Donostia International Physics Center, 20018 San Sebastián/Donostia, Basque Country, Spain

Low-energy electron microscopy (LEEM) is a technique that allows for in situ monitoring of surface processes in reactive environments at nanometer length scales and at video rates. While the qualitative interpretation of the image sequences for simple enough systems appears quite straight-forward, understanding the detailed structure in nanoscale multicomponent systems such as, e.g., those found in oxide heteroepitaxy and inverse model catalysts, is much more intricate. A possible solution to this conundrum is the analysis of the dependence of the specular electron reflectivity on the kinetic energy of the incident electrons, also known as the (00)-beam  $I(V)$  curve in low-energy electron diffraction (LEED). This  $I(V)$  curve contains detailed information on the geometric and electronic structure of the probed sample surface. In low-energy electron microscopy experiments, which typically are performed at fields of view in the range of a few microns or more in diameter, this dependence can be used for tying together mesoscale morphological observations and dynamics with nanoscale knowledge on atomic and electronic structure [1]. Furthermore,  $\mu$ LEED experiments can be conducted using electron beam diameters down to a few hundred nanometers, providing local insights into surface periodicity, morphology, and atomic structure.

In this contribution, we will use the capabilities of  $I(V)$ -LEEM and  $\mu$ LEED for real-time studies of the oxidation of the Ru(0001) surface by exposure to dioxygen ( $O_2$ ) and nitrogen dioxide ( $NO_2$ ) at elevated temperatures, allowing for characterizing and distinguishing different oxide orientations that concurrently evolve with increasing dose [2–4]. Interestingly, the  $RuO_2(100)$  orientation is shown to nucleate first for both types of oxidants whereas the well-known majority  $RuO_2(110)$  phase only develops at a later stage, concomitant with the growth of the (101) orientation. We will explain how this growth scenario, which at first glance appears counter-intuitive considering the surface free energies of the different oxide orientations, can be explained and how this complex oxidation behavior gives rise to roughening on the mesoscale. Furthermore, the morphology of the resulting oxide film is shown to strongly depend on the choice of oxidant due to strongly differing oxidation kinetics, demonstrating that the final structure very sensitively depends on the oxidation conditions.

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## Notes

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## **Resonant Scattering of (very) Low Energy Electrons from the Root-Three BiCu<sub>2</sub>/Cu(111) Surface Alloy**

**Bene Poelsema<sup>1</sup>, Michael Altman<sup>2</sup>, Raoul van Gastel<sup>1</sup>, Harold JW Zandvliet<sup>1</sup>, Arie van Houselt<sup>1</sup>**

<sup>1</sup>Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, P.O.Box 217, 7500AE Enschede, The Netherlands

<sup>2</sup>Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, P.R. China

Email: b.poelsema@utwente.nl

Strong evidence for bound state resonances of electrons is obtained for the ordered bismuth-copper surface alloy on Cu(111) using LEEM. LEEM intensity versus voltage curves obtained at normal incidence are measured at temperatures between 483 and 663 K. The position of the observed Bragg peak at 29.9 eV does not depend on temperature, in contrast to that of another peak which shifts from 23.2 eV to 21.0 eV with increasing temperature revealing an increasing relaxation of Bi within the terminating Bi-Cu-( $\sqrt{3}\times\sqrt{3}$ )R30° alloy. We also observe a strong, surprising intensity dip at 14 eV that remains at this position, irrespective of temperature. This position corresponds precisely to scattering into the in-plane  $G_{10}$  reciprocal lattice vector of the BiCu<sub>2</sub> root-3 alloy. Therefore, this dip provides evidence for bound state resonances, alternatively called selective adsorption, that involve coupling of the incident wave to in-plane channels via eigenstates of the image potential. The assignment is further corroborated by another, weaker but very persistent, intensity dip at 28 eV connected to a  $G_{11}$  reciprocal lattice position. Clear intensity dips are also observed at much lower energy, which only exist for finite size domains. These supernumerary dips are attributed to resonant electron scattering along high symmetry and also non-high symmetry directions far below the Ewald horizon. They emerge exclusively in the presence of ca. 10 nm sized ( $\sqrt{3}\times\sqrt{3}$ )R30° domains. We argue that selective adsorption of electrons should be a quite general phenomenon and LEEM is very sensitive to observe these features.



## Notes

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## Transport Measurements on Epitaxial Bi<sub>1-x</sub>Sb<sub>x</sub> Thin Films Grown on Si(111)

**Julian Koch, Philipp Kröger, Herbert Pfnür, Christoph Tegenkamp**

Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS,  
Appelstr. 2, 30167 Hannover

The alloy Bi<sub>1-x</sub>Sb<sub>x</sub> can be tuned to be either topologically trivial or non-trivial by changing the relative concentrations of Bismuth and Antimony [1]. In this study we present surface transport measurements performed on non-trivial Bi<sub>1-x</sub>Sb<sub>x</sub> films. Thin films grown by in-situ co-deposition on Si(111) substrates are used in order to reduce bulk contributions and to provide the possibility of nanostructuring. The morphology was controlled by 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 4, 8, 16 and 24 nm. The analysis of the temperature dependency allowed us to distinguish between different transport channels originating from surface and bulk bands as well as impurity states. At temperatures below 30 K the transport is mediated by surface states while at higher temperatures activated transport via bulk channels sets in. The surface state conductivity and bulk band gaps can be tuned by the Sb-concentration and film thickness, respectively.

For films as thin as 4 nm the metallic transport signal attributed to the surface state vanishes in contrast to Bi(111) films grown under identical conditions. This is in accordance with measurements on Bi<sub>2</sub>Se<sub>3</sub>, where a suppression of the metallic surface transport was observed for films with thicknesses of 6 nm or less, which is caused by an overlap of the wave functions of the surface and the interface, that leads to a hybridization gap in the Dirac dispersion [2, 3].

Compared to bulk materials, the bulk band gaps are increased by a factor of five due to quantum size effects, in accordance with theory [4]. With increasing Sb concentration the conductivity of the surface transport channel increases. This is in line with recent ARPES measurements showing increased filling factors of the surface bands [5].

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## Notes

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## **Photoemission Tomography: Imaging the Orbitals of Adsorbed Molecules with Angle Resolved Photoemission**

**Michael G. Ramsey**

Institute of Physics, Karl-Franzens University Graz, Austria

Here it will be shown that the apparently complex angular distribution of valence band photoemission from molecular films can be simply and quantitatively predicted from a Fourier transform of initial state wavefunctions. This suggests, contrary to popular belief, that overall dependence of the photocurrent can be well accounted for by assuming a plane wave for the final state. The imaging of the photoemission angular distribution together with an analysis based on the plane wave final state approximation is becoming known as orbital or photoemission tomography

While reconstruction of real space orbitals is the most spectacular demonstration of photoemission tomography it's power lies in the ability it gives to identify photoemission features to particular states and molecular geometries. This will be demonstrated for a variety of orbitals of the proto-typical pi conjugated molecules pentacene, sexiphenyl and PTCDA on a number of substrate surfaces. For adsorbate monolayers it will be shown how photoemission tomography can be used to determine molecular geometries, unambiguously determine the orbital energy ordering, gain insight into the nature of the surface chemical bond and image the orbitals in real space.

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## Notes

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## **Growth of CuPc and NTCDA on Cu(001) Studied by LEED and LEEM**

**Jana Wolters, Jonas van Bebber, Janina Felter, Markus Franke,  
Caroline Henneke, Christian Kumpf**

Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and  
Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology

A good understanding of the interactions between organic molecules and metal surfaces is essential for improving the performance of organic (opto-)electronic devices as well as for fundamental studies of thin organic films and metal-organic interfaces. In this context the first organic layer adsorbed on the metal substrate is of special importance since it is serving as a template for further growth and directly influences the physical properties of the interface.

We report a combined LEED and LEEM study on two model systems, Cu-Phthalocyanine (CuPc) and 1,4,5,8-naphthalene-tetracarboxylic-dianhydride (NTCDA) on the Cu(001)-surface. Growth and ordering phenomena were investigated in-situ and in real-time in both real and reciprocal space. For both systems, we identified several different phases occurring at different temperatures and coverages. One of them exhibits an unexpected behavior that resembles dendritic growth.

## Notes

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# Surface Crystallography of PTCDA on Ag(100) by LEED-IV Using Fourier Coefficients

**Ina Krieger<sup>1,3</sup>, Georg Held<sup>2</sup>, Christian Kumpf<sup>3</sup>, Moritz Sokolowski<sup>1</sup>**

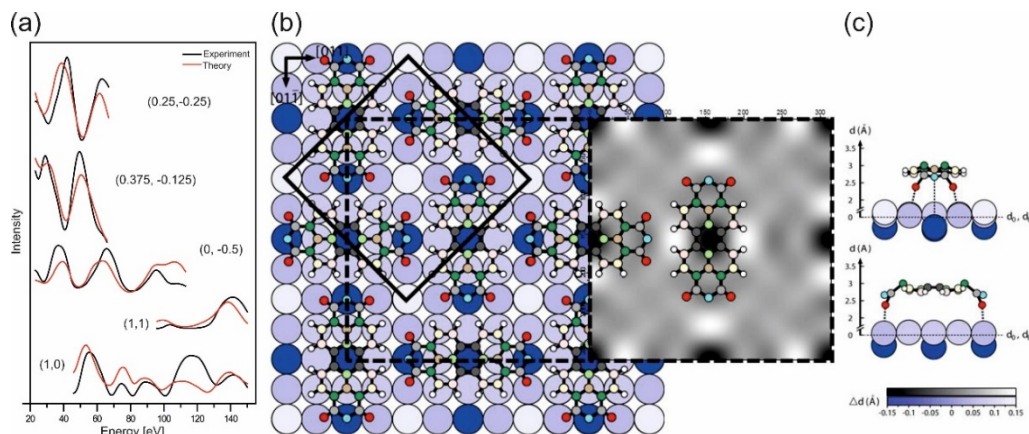
<sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Bonn, 53115 Bonn, Germany

<sup>2</sup>Department of Chemistry, University of Reading and Diamond Light Source, UK

<sup>3</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52428 Jülich, Germany

Here we will report on a LEED-IV analysis of PTCDA on Ag(100). Using data from different angles of incidence and optimizing the program code we were able to overcome challenges given by the limitations of the experimental data set and the calculation times required for the complex and large unit cell. In our first analysis, pronounced vertical out-of-plane displacements of individual atoms within the molecule and the Ag layers were fitted, which required further critical analysis. Thus, in a second step, the distortion of the PTCDA molecule and the buckling of the Ag surface were described by Fourier coefficients taking into account the symmetry of the system [1]. The idea is to stabilize the distortions and to reduce the number of free fitting parameters by restriction to low order coefficients.

Using Fourier components as fitting parameters we obtain, at present, a good Pendry R-factor of about 0.25. The calculation is based on a unit cell containing 156 atoms and experimental curves for five angles of incidence with an energy-to-parameter ratio over 300 eV. We were able to derive the vertical distortions of the oxygen atoms in the functional group and the buckling of the Ag surface in rather good agreement with earlier results from DFT and NIXSW studies [2]. In particular we found upward shifted Ag atoms under the carboxylic oxygen atoms and downward shifted Ag atoms below the PTCDA perylene core center. Supported by the DFG.



**(a)** Set of experimental (black) and calculated (red) LEED-IV curves for PTCDA/Ag(100) and **(b)** top and **(c)** sectional views of the adsorption geometry of PTCDA/Ag(100) as calculated by LEED-IV. Ag atoms are shown in different shades of blue to indicate the vertical deviation  $\Delta d$  from their position in the relaxed uncovered surface (dashed line,  $d_0$ ); H atoms are shown in white,  $O_{\text{carb}}/O_{\text{anhyd}}$  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,  $d_B$ ). The primitive unit cell (full lines) and the conventional  $c(8 \times 8)$  unit cell (dashed lines) are indicated. The inset in (b) illustrates the modulation of the first Ag layer described by the start parameters of the Fourier coefficients. This is shown for the  $c(8 \times 8)$  unit cell.

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## Notes

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## Quantitative LEED Studies on Si(111)-(5x2)-Au

**Andreas Alexander, Frederic Timmer, Joachim Wollschläger**

Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück

The (5x2)-Au reconstruction on Si(111) has been in the focus of research for nearly 50 years now. Lately, in particular as a prototype for one-dimensional (1D) metallic chain structures. In order to understand the physical properties accompanying these 1D chains a profound knowledge of the atomic structure is needed. Historically, a plethora of atomic structures (EBH [1], AN [2], KK [3]) with varying Au coverages were discussed. More recently Shirasawa *et al.* [4] were able to show that Surface X-ray Diffraction experiments favor the KK-model slightly. Due to the higher surface sensitivity of Low Energy Electron Diffraction (LEED) as compared to SXRD we carried out quantitative LEED experiments in order to assess this observation.

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# Growth and Structure of Sn Deposited on Ge Wetting Layers Grown on Si(001)

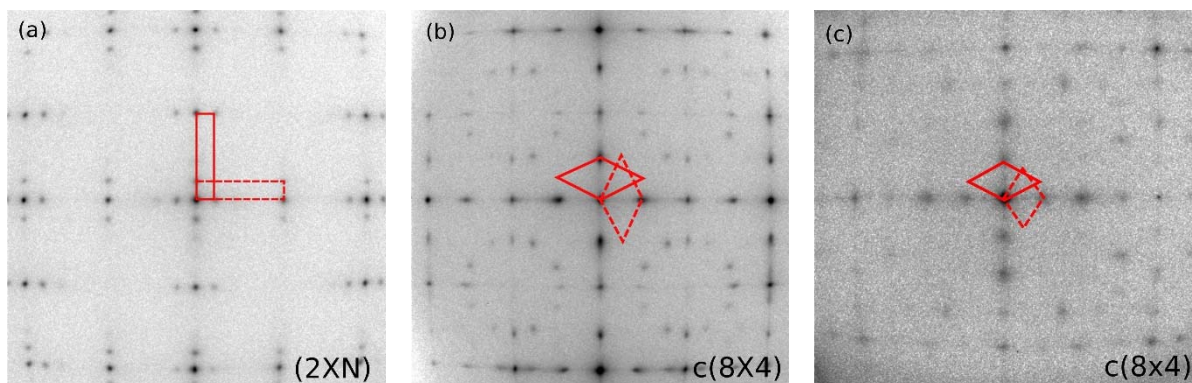
**Nicolas Braud, Thomas Schmidt, Jens Falta**

Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

SnGe is expected to play an important role in optoelectronic and in future Ge device modules integrated into CMOS technologies due to its potentially indirect to direct bandgap transition [1] and its higher carrier mobility compared to Ge [2]. SnGe is also offering new possibilities concerning strain engineering due to the large lattice mismatches between Sn and Ge [3].

Here we present SPALEED investigations of the structure of Sn grown by solid-phase epitaxy on Si(001) and on Ge wetting layers. The latter were deposited by molecular-beam epitaxy on Si(001) at 465°C. The Sn adsorption was carried out at room temperature, followed by annealing at 570 to 680°C for 2 min. While there exist a few studies [1] of the Sn/Si(001) system, the surface reconstructions of Sn on Ge(001) have not been investigated so far. Hence, we present the first surface science study of this material system, using Ge template layers grown on Si(001) as substrates.

In agreement to literature [1], we were able to identify four different superstructures for the Sn/Si(001) system: We observed a  $c(4 \times 4)$ , a  $(5.5 \times 2)$ , a  $c(8 \times 4)$  and a  $(5 \times 1)$  reconstruction for 0.24, 0.44, 0.80, and 1.05 ML of Sn, respectively, after deposition at room temperature and subsequent annealing between 570 and 680°C. The  $c(8 \times 4)$  to  $(5 \times 1)$  phase transition has been found to be reversible by a short heating-cooling cycle. For Sn adsorption on Ge wetting layers, a similar behavior has been observed and will be discussed in detail.



**Figure 1:** SPALEED patterns after (a) Ge deposition on Si(001) at 465°C, (b) Sn deposition at room temperature on Si(001), and (c) deposition of Sn on a Ge wetting layer, followed by annealing at 570°C for 2 minutes. In each frame, the red tetragons indicate the primitive reciprocal unit mesh, occurring in two 90° rotational domains.

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## Growth of PTCDA Domains on an Epitaxial Hexagonal Boron Nitride Monolayer

Christine Brölke<sup>1</sup>, Timo Heepenstrick<sup>1</sup>, Ina Krieger<sup>1</sup>, Moritz Sokolowski<sup>1</sup>,  
Sergey Subach<sup>2</sup>

<sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstrasse 12,  
53115 Bonn, Germany

<sup>2</sup>Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

Epitaxial monolayers of hexagonal boron nitride (hBN) on different metal surfaces are of high interest as a two-dimensional insulating substrate as well as templates for the formation of epitaxial layers of organic molecules [1]. Here, we report a structural analysis of one monolayer of the model molecule PTCDA on hBN/Cu(111) by spot profile analysis low energy electron diffraction (SPA-LEED).

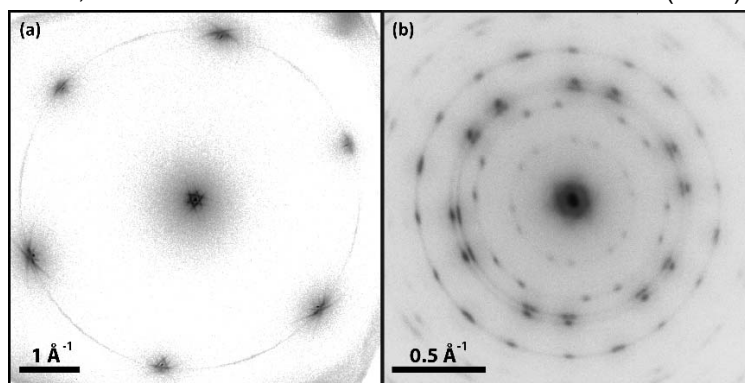
hBN grows on the Cu(111) surface in an incommensurate structure with a lattice mismatch of 2.3 % corresponding to an unstrained hBN layer. The films show rotational mosaicity, however, the majority of the hBN domains are in or close to alignment with the unit cell vectors of the Cu(111) surface ( $\pm 2^\circ$ ). The SPA-LEED patterns show detailed satellite structures which can be explained by multiple electron scattering.

The SPA-LEED pattern of one monolayer PTCDA on this hBN layer shows an azimuthal broadening of the PTCDA spots due to the rotational mosaicity of the hBN substrate. The PTCDA molecules form an ordered herringbone structure as in the (102)-plane of the bulk crystal [2]. The lattice constants of the PTCDA layer on hBN deviate only slightly ( $< 3\%$ ) from the lattice constants of the (102) plane of the  $\alpha$ -modification of the bulk crystal with  $a = (19.36 \pm 0.09)$ ,  $b = (12.1 \pm 0.2)$  Å.

A comparison with PTCDA layers on the Ag(111) and Cu(111) surfaces reveals a decrease in commensurability (PTCDA/Ag(111) is commensurate [2], PTCDA/Cu(111) [3] shows point-on-line commensurability and PTCDA/hBN/Cu(111) is incommensurate) with decreasing misfit with respect to the PTCDA bulk lattice constant. This points to decreasing strength of interaction between the PTCDA and the substrates going from Ag(111) to Cu(111), and hBN.

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**Figure 1:** (a) SPA-LEED pattern of hBN/Cu(111) at 70.7 eV.  
(b) SPALEED pattern of PTCDA/hBN/Cu(111) at 30.4 eV.

## The Effect of Adsorbates on the Transport Characteristics of Au Chains on Vicinal Si(hhk) Surfaces

**Frederik Edler<sup>1</sup>, Ilio Miccoli<sup>1</sup>, Jan Philipp Stöckmann<sup>1</sup>, Herbert Pfnür<sup>1</sup>,  
Christoph Tegenkamp<sup>1</sup>**

<sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover,  
Appelstraße 2, 30167 Hannover, Germany

Atomic chain ensembles grown by self-assembly are prototype 1D systems with outstanding electronic properties for fundamental research studies such as Peierls driven metal to insulator phase transition (MIT) or dimensional crossover from Fermi to Luttinger liquid behavior. However, it is well known that these properties are strongly affected by imperfections or near surface modifications, e.g. the interwire coupling as well as MIT temperature of indium chains on the Si(111)-4x1 surface is strongly dependent on the presence of oxygen-mediated defects [1].

Here, we present a systematic study on the transport properties of chains of gold atoms self-assembled on vicinal Si(hhk) surfaces via a multi-tip STM/SEM system and the rotational four-point-probe square method [2]. The transport characteristics of various Au/Si(hhk) systems, i.e. conductivity values along and perpendicular to the chains as well as the anisotropy ratio, were carefully studied and correlated with the miscut-angle of the substrate, the gold coverage and the Au-induced surface refaceting (investigated by LEED). In addition, in-situ adsorption experiments with molecular oxygen were performed to tune and modify the intra- and interwire couplings within the ensemble. Most strikingly, the Au/Si(553) system showed for Au chain ensembles prepared with different Au coverages very different transport characteristics as exposed to oxygen. While the 0.48 ML Au on Si(553) turns out to be extremely robust and almost unaffected (up to 60 Langmuir), the 0.19 ML phase, where Au adsorbs on every next but Si terrace [3], reacts strongly as seen by the exponential like decrease its conductivity components. We will discuss the different transport findings in terms of the different building blocks (Au chains, Si-adatom chain, Si edge) found for the Au/Si(hhk) systems [4].

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## **$\mu$ ARPES on Molecular Adsorbate Systems: Proof of Principle Experiments for Single Domain K-Space Mapping**

**Janina Felter<sup>1,2</sup>, Jana Wolters<sup>1,2</sup>, Markus Franke<sup>1,2</sup>, Caroline Henneke<sup>1,2</sup>,  
Christian Kumpf<sup>1,2</sup>**

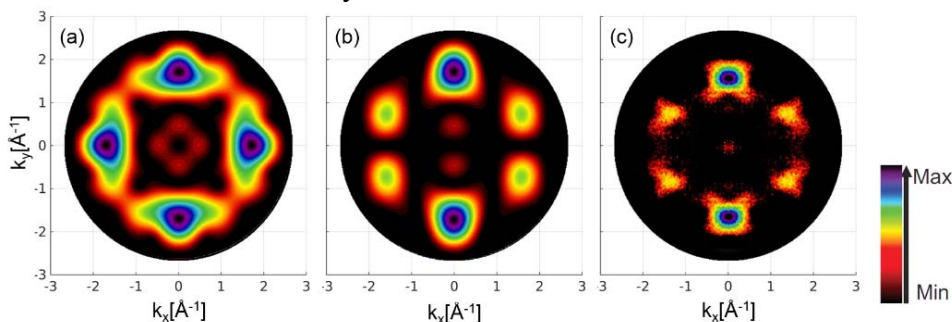
<sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany

<sup>2</sup>Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology

Email: j.felter@fz-juelich.de

The adsorption of organic molecules on metal surfaces is of highest relevance for applications in the field of organic electronics. Therefore, fundamental studies are frequently performed as well. Both structural (e.g. nucleation and layer formation) and electronic properties (band structure, electronic level alignment, interaction across the interfaces, etc.) are in the focus of present investigations. The technique of k-space mapping became particularly interesting for investigating the latter aspects, and is routinely performed with electron spectroscopes located at synchrotron beamlines and in home-based laboratories. Such experiments usually have no significant spatial resolution, and hence – in the particular case of molecular adsorbates – suffer from the fact that the resulting data averages over many surface domains which complicates the data analysis.

Here, we demonstrate that by using a LEEM/PEEM instrument and a conventional VUV lab source, one is able to perform k-space mapping on a single domain of a molecular adsorbate system by recording ARPES data of micrometer sized surface areas ( $\mu$ ARPES). As a model system, we selected the aromatic molecule 1,4,5,8-naphthalene-tetracarboxylic-dianhydride (NTCDA) on the Cu(001)-surface. By in-situ and real-time investigations using LEEM and  $\mu$ LEED, we identified two different phases occurring at different temperatures. One of them exhibits rather large molecular domains caused by an unexpected, dendritic-like growth behavior. Therefore, it represents an excellent prototype system for PEEM-based  $\mu$ ARPES and k-space imaging. In Figure 1, we compare calculated and measured constant binding energy (CBE) maps for the case of domain averaging (a) and single-domain resolution (b, c). We believe that this technique can significantly improve the quality of orbital tomography results, especially for adsorbate systems on highly symmetric (111) surfaces and heteromolecular systems.



**Figure 1:** (a, b) Theoretical CBE maps of the LUMO of NTCDA on Cu(001), calculated for the average of both possible domains (a) and for only one domain (b). (c) Corresponding measured CBE map of a single domain.

### **Acknowledgement**

The authors thank Daniel Lüftner from the Technical University of Graz for calculating the CBE maps.

# Growth and Characterization of Thin VO<sub>2</sub> Films on TiO<sub>2</sub>(110)

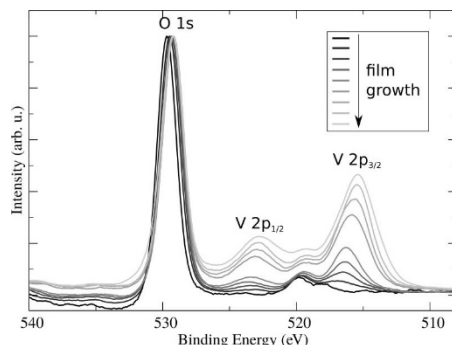
**Simon Fischer, Jon-O. Krispeneit, Jan I. Flege, and Jens Falta**

Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

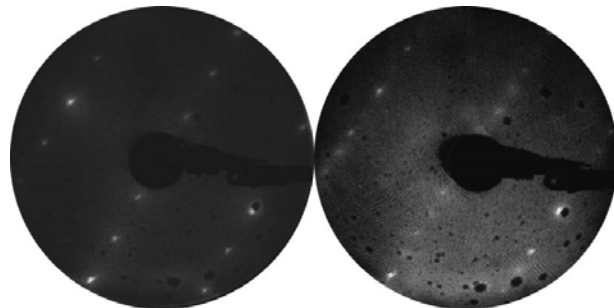
With VO<sub>2</sub> exhibiting a temperature-induced metal-insulator transition (MIT), thin film growth of this correlated material is of interest for various applications such as switching devices and sensors [1, 2]. The MIT is accompanied by a structural change with the high-temperature phase being rutile and metallic. The monoclinic low-temperature phase is insulating on account of vanadium ion dimerization [3]. By using TiO<sub>2</sub> substrates, the MIT temperature can be tuned because of the resulting strain. However, because of the multivalent nature of vanadium, a number of different vanadium oxides can form, depending on substrate, oxidation source and growth temperature [4].

We have grown vanadium oxide films by plasma-assisted reactive molecular beam epitaxy. Vanadium was deposited continuously and the sample was subjected to varying doses of atomic oxygen. Between growth cycles, x-ray photoelectron spectroscopy was employed to identify the vanadium oxidation state from the position of the V 2p<sub>3/2</sub> peak [5, 6] and the film thickness was calculated by Ti 2p<sub>3/2</sub> substrate peak attenuation between growth cycles.

Apparently, high oxidant doses favor polycrystalline V<sub>2</sub>O<sub>5</sub> growth in thicker films, thus increasing contact resistance, while VO<sub>2</sub> phases might still exist in the interface area. Lower doses that still sufficiently oxidize the film lead to epitaxial VO<sub>2</sub> growth with low surface roughness, as confirmed by scanning tunneling microscopy. Several surface reconstructions were observed by low energy electron diffraction (cf. figure 2). Ex situ, measurements of temperature-dependent resistance further characterize the film quality.



**Figure 1:** XPS spectra of sample subjected to low plasma doses. V 2p<sub>3/2</sub> peak shift indicates a gradual change from V<sub>2</sub>O<sub>5</sub> to VO<sub>2</sub> during growth.



**Figure 2:** Left: substrate LEED pattern. Right: LEED pattern observed during growth.

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## Crystal Morphology Investigation of LiFePO<sub>4</sub> Microparticles Using AFM and First-Principles Calculations

**Kevin Gradwohl<sup>1</sup>, Peter Benedek<sup>2</sup>, Maxim Popov<sup>3</sup>, Jürgen Spitaler<sup>3</sup>, Maksym Yarema<sup>2</sup>, Vanessa Wood<sup>2</sup>, Christian Teichert<sup>1</sup>**

<sup>1</sup>Institute of Physics, Montanuniversität Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

<sup>2</sup>Laboratory of Nanoelectronics, ETH Zürich, Gloriastrasse 35, CH-8092 Zürich, Switzerland

<sup>3</sup>Materials Center Leoben Forschung GmbH (MCL), Roseggerstraße 12, 8700 Leoben, Austria

Olivine structure LiFePO<sub>4</sub> (LFP) is one of the most promising candidates for cathode materials in large scale applications. We investigated the geometry of faceted LFP microparticles by atomic force microscopy (AFM). Different particle shapes were obtained by changing the precursor concentration and introducing surfactants in a modified hydrothermal synthesis process proposed by Ref. [1]. With the quantitative AFM surface information (edge angles and facet tilts) we were able to determine the Miller indices of each facet by an error minimization technique. The facet orientations have been compared to previous first-principles studies [2]. All facets observed were low surface energy facets according to Ref. [2] except for (210) which was not considered there. We calculated the surface energy of (210) within density functional theory in the generalized gradient approximation (GGA) + U framework and found that the missing facet contributes about 2.5% to the total area of the Wulff-Plot.

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## Spin Correlations in the Si(553)-Au Nanowire System

**Bernd Hafke**, Tim Frigge, Tobias Witte, Boris Krenzer,  
Michael Horn-von Hoegen

Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen,  
Lotharstr. 1, 47057 Duisburg, Germany

To study the microscopic mechanism of formation, stabilization, and interaction in low dimensional systems we used Si(553) as vicinal surface to enforce the nucleation of Au into one dimensional wires. Deposition of 0.5 ML Au results in the formation of one pair of 1D Au atomic chains per Si terrace. These chains are slightly dimerized along the terrace direction, thus exhibiting a twofold periodicity. These metallic wires are structurally terminated by Si step edge atoms, which show a threefold periodicity of the Si atoms along the rows. Theory calculations predicts an antiferromagnetic spin ordering of every third Si step edge atom [1].

The long-range interaction of the twofold and threefold periodicity is investigated by spot-profile analysis in SPA-LEED at a sample temperature of 80 K. The strict twofold periodicity of the Au atoms is not correlated between adjacent wires. In contrast the threefold ordering of the Si spins exhibits a clear short range order perpendicular to the Au wires, i.e., the direction perpendicular to the terraces. Both results support the structure model where the interrow correlation of the Si step edge atoms is mediated by the spin-spin interaction of adjacent Si step edge atoms.

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## **Sub 400 fs Temporal Resolution in Reflection High-Energy Electron Diffraction at Surfaces for Phase-Transition Studies**

**Bernd Hafke, Tim Frigge, Tobias Witte, Boris Krenzer,  
Michael Horn-von Hoegen**

Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen,  
Lotharstr. 1, 47057 Duisburg, Germany

In time resolved reflection high energy electron diffraction an ultrashort electron pulse probes the surface at grazing incidence to ensure surface sensitivity. At energies of 30 keV the electrons travel at 1/3 of the speed of light and require 20 ps to traverse a typical sample width of 2 mm. For pump-pulses at normal incidence all sample areas are excited simultaneously. This geometric velocity mismatch limits the overall experimental temporal resolution. Employing a tilted pulse front scheme for the laser excitation we are able to overcome this limitation and obtain a temporal resolution of 600 fs when probing the entire sample width. Reduction of the electron number per pulse and probing only a narrow part of the sample further improves the temporal resolution to less than 400 fs. No electron pulse compression scheme was used for this experiment. Temporal broadening due to vacuum dispersion on the 8 cm distance between photocathode and sample is minimized by the narrow initial electron energy spread of only 100 meV of our back illuminated Au photocathode.

An optimized electron gun design ensures a vertical coherence length of more than 50 nm. An integration time of 10 s is sufficient for good statistics for each delay time step, i.e., a diffraction movie with 100 frames at time steps of 50 fs is recorded in less than 30 min. This emphasizes the advanced signal-to-noise ratio opening a new field of research due to time-resolved, surface-sensitive spot-profile analysis.

## The surface reconstruction of Pt(001) quantitatively revisited

Rene Hammer<sup>1</sup>, Klaus Meinel<sup>1</sup>, Oliver Krahn<sup>1</sup>, Stefan Förster<sup>1</sup>, Wolf Widdra<sup>1,2</sup>

<sup>1</sup>Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

<sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

The complex hexagonal reconstructions of the (001) surfaces of platinum and gold are under debate since decades. Recently, we combined the high resolving power of scanning tunneling microscopy (STM) and spot profile analysis low energy electron diffraction (SPA-LEED), supported by LEED simulations based on a Moiré approach, to show that the Au(001) reconstruction consists of two rotational domains of a commensurate  $c(28 \times 48)$  superstructure [1].

Here, we present a high-resolution study of the hexagonal reconstruction of Pt(001). Annealing to 850 °C yields the formation of a hexagonal top layer where closed packed atomic rows follow the [110]-like directions of the square Pt(001)-(1x1) substrate. This non-rotated hex approaches a Moiré-like  $c(26 \times 118)$  superstructure which is in commensurate registry with the quadratic substrate.

Sample annealing at 920 °C yields a continuous rotation of the hex layer between an angle area of  $0 - 0.7^\circ$  and  $+ 0.7^\circ$ . Within this angle area, no favored rotation angles were observed. During rotation, the internal structure of the  $c(26 \times 118)$  hex is maintained due to its strong internal compression. At temperatures around 1080 °C, the non-rotated hex coexists with a hex which is rotated by about  $0.75^\circ$ . Annealing at temperatures around 1120 °C yield a locking of the hex in fixed rotation angles of  $0.77^\circ$ ,  $0.88^\circ$ , and  $0.94^\circ$ . For temperatures around 1170 °C, the rotated Pt(001)-hex-R $0.94^\circ$  is identified as the energetically most favored reconstruction structure of Pt(001). It is described as incommensurate structure which might have a point-on-line registry with the Pt(001) substrate.

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## Growth of (100) Oriented Ceria Nanostructures on Close-Packed Transition Metal Surfaces

**Jan Höcker<sup>1</sup>, Tomáš Duchoň<sup>2</sup>, Sanjaya D. Senanayake<sup>3</sup>, Jens Falta<sup>1</sup>, Jan I. Flege<sup>1</sup>**

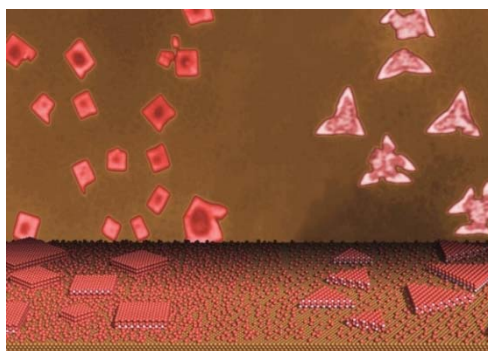
<sup>1</sup>Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

<sup>2</sup>Department of Surface and Plasma Science, Charles University in Prague, 18000 Praha, Czech Republic

<sup>3</sup>Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, USA

The epitaxial growth of cerium oxide on transition metal surfaces has become a very popular approach to create model catalyst architectures as, e.g., nanoparticles or ultrathin films for the investigation of its peculiar chemical properties. Typically, the emerging ceria adopts the (111) surface orientation, which is usually considered the most stable from a thermodynamic point of view. Intriguingly, under more realistic conditions also more open surface orientations are found, e.g., in the case of cuboidal nanoparticles, which may exclusively be terminated by (100) surfaces. Furthermore, these surfaces have been shown to exhibit chemical behavior very different from the more prominent (111) orientation [1]. However, for a selective study of the individual catalytic properties of the different ceria surfaces employing the powerful tools of surface science their controlled preparation under near-ultrahigh-vacuum conditions is highly desirable.

Here, a novel and simple method is presented for the preparation of a well-defined  $\text{CeO}_2(100)$  model system on  $\text{Cu}(111)$  based on the adjustment of the Ce/O ratio during growth (Fig. 1) [2]. The method yields micrometer-sized, several nanometers high, single-phase  $\text{CeO}_2(100)$  islands with controllable size and surface termination that can be benchmarked against the (111) nanostructured islands on  $\text{Cu}(111)$ . Furthermore, we demonstrate the ability to adjust the Ce to O stoichiometry from  $\text{CeO}_2(100)$  (100%  $\text{Ce}^{4+}$ ) to  $\text{c-Ce}_2\text{O}_3(100)$  (100%  $\text{Ce}^{3+}$ ), which can be readily recognized by characteristic surface reconstructions observed by low-energy electron diffraction. The discovery of the highly stable  $\text{CeO}_x(100)$  phase on a close packed metal surface represents an unexpected growth mechanism of ceria on  $\text{Cu}(111)$ , which will be contrasted with ceria(100) nanoparticle growth on  $\text{Ru}(0001)$  at temperatures above 1100 K [3].



**Figure 1:** Controlling the ceria orientation and morphology on  $\text{Cu}(111)$  during growth by tuning the cerium-to-oxide-ratio.

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## In-Situ Characterization of Ultrathin Praseodymia Films on Ru(0001)

**Jon-O. Krisponeit<sup>1</sup>, Jan Höcker<sup>1</sup>, Andreas Schaefer<sup>2</sup>, Julian Cambeis<sup>1</sup>, Alexei Zakharov<sup>2</sup>, Yuran Niu<sup>2</sup>, Jens Falta<sup>1</sup>, Jan I. Flege<sup>1</sup>**

<sup>1</sup>Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

<sup>2</sup>MAX IV Laboratory, Lund University, Lund, Sweden

Praseodymia exhibits a complex phase diagram covering the range from the sesquioxide  $\text{Pr}_2\text{O}_3$  to the fully oxidized  $\text{PrO}_2$  [1]. Due to its even higher oxygen mobility and its large oxygen storage capacity, it should be considered as an equally promising catalyst material like ceria, a closely related and prominent catalyst. As an inverse catalyst model system, ceria microparticles can be grown in excellent crystalline quality on the Ru(0001) surface [2], stimulating the presented approach to grow ultrathin praseodymia films on ruthenium single crystals.

We prepared  $\text{PrO}_x/\text{Ru}(0001)$  films by reactive molecular beam epitaxy and studied their structural, morphological and chemical properties in-situ. By low energy electron microscopy (LEEM), we observed a nucleation of triangular islands along the Ru(0001) step edges which coalesce forming band-like structures. Furthermore, x-ray absorption spectroscopy was employed in imaging mode (XAS-PEEM) to characterize the local chemical composition of the praseodymia islands, indicating the growth of  $\text{Pr}_2\text{O}_3$ .

Finally, we recorded  $\mu$ -LEED images with three-fold symmetry and observed atomic step heights of 0.3 nm on the top facets of the islands via atomic force microscopy. These results allow the praseodymia islands to be structurally identified as hexagonal  $\text{Pr}_2\text{O}_3$  (0001). In  $\mu$ -LEED and dark-field LEEM we revealed the formation of rotational domains under  $\approx 12^\circ$  with respect to the substrate orientation. The angles of rotation can be explained as low-strain registries between the praseodymia film and the substrate.

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## Surface Transport on Thin Semi-Metallic Films: The Role of Film Thickness and Magnetic Impurities

**Philipp Kröger<sup>1</sup>, Marianna Siemens, Christoph Tegenkamp<sup>1</sup>, Herbert Pfnür<sup>1</sup>**

<sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The semi-metal bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentrations and high carrier mobilities. Thereby, epitaxial growth of high-quality thin films opens new pathways to tailor the electronic properties further, e.g. by quantum confinement [1] and alloy formation [2], giving rise to topologically non-trivial states in this material class. In this study we concentrate on Bi films grown on Si(111). Thin Bi(111) films become semiconducting, thus the peculiar spin texture of the surface states, induced by the Rashba effect, can be studied directly by temperature and magnetic field dependent transport.

The conductance  $G$  at low temperature is mainly governed by surface states while at higher temperatures activated transport from bulk channels sets it. We have carefully analyzed the  $G(T)$  - behavior for variously thick films. With decreasing film thickness, the bulk gap increases, as expected due to the quantum size effect. However for thinner films the gap decreases and finally the surface states overlap with bulk bands. The reason is an interface-interface interaction which renormalizes strongly the Fermi surfaces [1].

Moreover, magnetic impurities Cr, Co, Fe and Mn, in the range of a few percent of a monolayer were added to probe the scattering behavior of the spin-polarized surface channels by magneto-conductance. The adsorption of all of these elements is accompanied by charge transfer (0.3 - 0.5h/atom) and strong spin-orbit scattering, which results in a transition of strong weak anti-localization to weak localization. The strength of spin orbit scattering differs among the magnetic atoms and is directly connected to their magnetic moment in the adsorbed state [3].

**Keywords:** semi-metallic films, surface transport, magnetic impurities

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## **Au-chains Grown on Ge(100): A Detailed SPA-LEED study**

**Timo Lichtenstein<sup>1</sup>, Heiko Teiken<sup>1</sup>, Herbert Pfnür<sup>1</sup>, Joachim Wollschläger<sup>2</sup>,  
Christoph Tegenkamp<sup>1</sup>**

<sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover

<sup>2</sup>Fachbereich Physik, Universität Osnabrück

Ge(100) is known as a substrate for self-organized growth of one-dimensional quantum wires by adsorption of Au. Those wires were shown to exhibit spectroscopic signatures of strong electronic correlation. As shown by C. Blumenstein *et al.* (Nature 7, 776) the signatures of this proposed Luttinger liquid behavior depends crucially on the quality of the ensemble and, consequently, on the quality of the Ge(100) sample prior to adsorption. Furthermore, the atomistic structure of these wires is still controversially discussed.

In this study, the morphology has been investigated by means of spot profile analysis low energy electron diffraction (SPA-LEED). We measured systematically the properties on variously prepared surfaces. From G(S)- and H(S)-analyses on ex-situ chemically treated Ge-samples followed by in-situ thermal annealing reveal step heights of 1.42 Å with average terrace lengths around 20 nm and an RMS-roughness of 1.3 Å. Carrying out multiple in-situ Ar<sup>+</sup>-sputtering and high-temperature annealing cycles, the terrace width increases to around 100 nm, the roughness slightly decreases.

After the growth of the Au-wires, the G(S)-curves feature additional structures corresponding to step heights of 1.8 Å which we suggest to be due to the interference of the reshaped gold induced surface structure with the underlying bulk. The detailed analysis of diffraction profiles favors strongly to the model of an 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 penetrates into subsurface positions stabilizing the adsorbate-induced surface structure.

## **Two-Dimensional Crossover in One-Dimensional Plasmons in Si(hhk)-Au: The Power of an Energy Sensitive EELS-LEED**

**Timo Lichtenstein, Christoph Tegenkamp, Herbert Pfnür**

Institut für Festkörperphysik, Leibniz Universität Hannover

For future plasmonic devices the understanding of low-dimensional collective excitations is indispensable. Nevertheless, although basic theories of the properties of low-dimensional plasmons exist for many years, their description and predictions of the behavior is still rather unsatisfactory. Several fundamental aspects of the influence such as, e.g. many-body effects as well as Coulomb screening are still rather unexplored. Additionally, (quasi-)one-dimensional (1D) electronic systems show exceptional transport properties such as Peierl's transitions or Tomonaga-Luttinger liquid (TLL) behavior, that have strong influence of the plasmonic properties.

For quasi-one-dimensional structures Au induced wires on regularly stepped Si(hhk) offer the perfect playground with their varying terrace widths. Therefore, the systems were prepared to a state, where each of these terraces hosts a gold chain.

For our investigations, the wire quality was checked with spot profile analysis in low energy electron diffraction (SPA-LEED). A combination of an electron energy loss spectrometer (EELS) and SPA-LEED providing both high energy and momentum resolution gave access to the plasmon dispersion.

Although 1D metallicity is observed, the plasmon dispersion strongly depends on a two-dimensional crossover: on the lateral distribution of the 1D electron density of states (DOS) within one terrace (intrawire correlation), as well as on the spacing of the wires (interwire correlation). This can quantitatively be described by a modified plasmon model for a wire array. We obtained effective widths which are considerably smaller than the terrace widths. A modulated DOS of comparable width can also be seen by tunneling spectroscopy. These effective widths seem to be influenced both by the structural motif, i.e. single or double chain, as well as by the terrace size.



## Domain Size Distribution of PTCDA on KCl(100) Determined by Analysis of LEED Profiles

**Christian Marquardt<sup>1</sup>, Alexander Paulheim<sup>1</sup>, Joachim Wollschläger<sup>2</sup>, Moritz Sokolowski<sup>1</sup>**

<sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn,  
Wegelerstrasse 12, 53115 Bonn

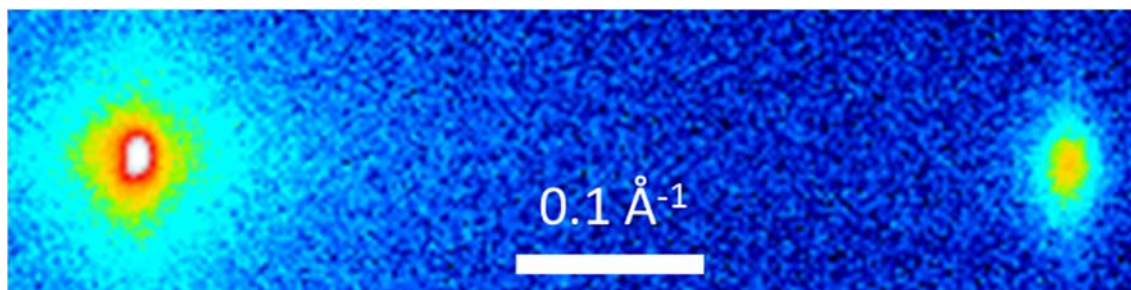
<sup>2</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

On the KCl(100) surface the organic dye molecule 3,4,9,10-perylenetetracarboxylic acid dianhydride (PTCDA) forms a monolayer with a commensurate ( $2\sqrt{2} \times 2\sqrt{2}$  R45°) brickwall structure. In this structure 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. The system shows a pronounced superradiant transition in fluorescence and excitation spectroscopy that is correlated with the number of coherently coupled molecules, which is limited by the lateral 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. This broadening is explained by finite-size effects, i.e., the size distribution of PTCDA domains [1].

Thus, we are interested in a precise determination of the PTCDA domain size distribution. For this purpose, we measured and analyzed high-resolution 2-dimensional LEED profiles. Since the profiles show no significant variations within several diffraction orders, domain boundaries are uncorrelated and inter-domain scattering can be neglected. The profiles show a pronounced diamond shape that indicates the presence of rectangular domains of the dimension of  $N_x \times N_y$  molecules with unpolar domain boundaries. Moreover, in a first approximation the profile shape in  $k_x$ -direction is independent from  $k_y$  and vice versa. Thus, it is possible to treat the directions independently from each other and to describe the 2-dimensional domain size distribution by a product of two 1-dimensional distributions. The 2-dimensional experimental LEED profile was calculated using a model domain size distribution and numerically convoluted with a theoretical 2-dimensional Gaussian instrument function. We find that 1-dimensional geometric distributions give the best fit to our data and yield an average domain size of  $11.8 \times 11.8$  molecules.

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LEED profiles of the specular spot (left) and the (1,0) spot (right) of the so-called brickwall (BW) phase of PTCDA on an epitaxial KCl(100) film on Ag(100).

## **Combined SPA-LEED and AES Studies of Tb Growth on Si(111) and Si(557) in the Monolayer Regime**

**Waldemar Schreiber , Frederic Timmer, Joachim Wollschläger**

Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück

Epitaxial thin films of rare earth silicides are of particular interest because of their possible applications and the large variety of different structures in the submonolayer range showing both planar 2D structures as well as quasi-1D wire-like structures. For instance, planar rare earth silicides serve as low-resistivity contacts to n-type Si due to the very low Schottky barriers while metallic nanowires might be used as interconnects or plasmonic waveguides [1-3]. Similar to other rare earth silicides (e.g. Dy silicide), depending on the deposited amount of rare earth elements, Tb silicide shows planar ( $\sqrt{3}\times\sqrt{3}$ ) structures as well as quasi-1D (5x2) (5x2) structures as reported from STM studies [4]. Therefore, we report here on the growth of Tb silicide on Si(111) to shed light on the growth kinetics of these different structures by means of Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED) and Auger Electron Spectroscopy (AES). In addition, its vicinal surface Si(557) has been investigated in the monolayer regime to investigate of atomic steps on the evolution of the different Tb silicide structures.

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## Ordered Superstructures of CuPc on Ag(110)

**Sergey. Soubatch<sup>1</sup>, Kathrin Schönauer<sup>1</sup>, Simon Weiss<sup>1</sup>, Vitaliy Feyer<sup>1</sup>, Daniel Lüftner<sup>2</sup>, Benjamin Stadtmüller<sup>1</sup>, Daniel Schwarz<sup>1</sup>, Tomoki Sueyoshi<sup>1</sup>, Christian Kumpf<sup>1</sup>, Peter Puschnig<sup>2</sup>, Michael G. Ramsey<sup>2</sup>, Stefan Tautz<sup>1</sup>**

<sup>1</sup>Forschungszentrum Jülich and Jülich Aachen Research Alliance (JARA), Germany

<sup>2</sup>Institute of Physics, NAWI Graz, Karl-Franzens University Graz, Austria

On the Ag(110) surface copper-phthalocyanine (CuPc) orders in two structurally similar superstructures, as revealed by low energy electron diffraction. Scanning tunneling microscopy shows that in both superstructures the molecular planes are oriented parallel to the surface and the long molecular axes, defined as diagonals of the square molecule, are rotated by  $\approx 32^\circ$  away from the high symmetry directions of the silver surface. Interestingly, at low temperature the majority of the CuPc monolayer is found in one of these two superstructures, while at room temperature it is dominated by another revealing the temperature driven phase transition. Thermodynamic analysis assisted by the results of the pair potential calculations demonstrates that the balance between two superstructures is governed by the competition between intermolecular interactions and molecule-substrate interfacial attractions. Furthermore, a symmetry analysis of experimental and theoretical constant binding energy maps of the photoemission intensity distribution in the reciprocal space points to a preferential occupation of one of the two initially degenerate lowest unoccupied molecular orbitals of CuPc. The lifting of the degeneracy of the LUMOs and the related reduction of the symmetry of the adsorbed CuPc molecule are attributed to an anisotropy in the chemical reactivity of the receiving Ag(110) surface.

## **Epitaxial Graphene Studied by ELS-LEED: Structure and Plasmonic Excitations**

**Christoph Tegenkamp**

The sheet plasmon in epitaxially grown graphene layers on SiC(0001) and the influence of surface roughness has been investigated in detail by means of low energy electron diffraction and electron energy loss spectroscopy. We show that the existence of steps or grain boundaries in this epitaxial system is a source of strong damping, while the dispersion is rather insensitive to defects. To first order, the lifetime of the plasmons was found to be proportional to the average terrace length and to the plasmon wavelength. A possible reason for this surprisingly efficient plasmon damping may be the close coincidence of phase (and group) velocities of the plasmons (almost linear dispersion) with the Fermi velocity of the electrons. Therefore, uncorrelated defects like steps only have to act as a momentum source to couple effectively plasmons to the electron–hole continuum.

## **Ultrathin Lead Films on Silicon (111): Growth and Lattice Response after Optical Excitation**

**Tobias Witte, Tim Frigge, Bernd Hafke, Boris Krenzer,  
Michael Horn-von Hoegen**

Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen,  
Lotharstr. 1, 47057 Duisburg, Germany

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  $\theta_{\text{Pb}} = 1/3$  ML Pb-coverage was prepared by desorption of a larger amount of Pb at 450 °C and further used as a template layer for deposition and azimuthal ordering of the films. Epitaxial growth is observed at temperatures below 100 K. LEED intensity oscillations reflects a layer-by-layer growth mode for coverages exceeding 3 ML. Up to 5 ML film thickness satellite spots surrounding the integer order spots are observed. These satellites vanish for  $\theta_{\text{Pb}} > 6$  ML. By deploying a G(S) analysis, the vertical layer distance is found to be increased by 10% at 3-5 ML thickness, and relaxes at 6ML. A quasi-G(S) analysis is introduced, which corroborates these findings. Additionally the layer distance is found to be varying for even and odd numbers of layers due to quantum size effects.

Furthermore time resolved RHEED has been employed to study the non-equilibrium dynamics of the phonon system after optical excitation. Using an infrared laserpulse the ultrathin lead films are excited, which leads to a loss in diffraction intensity due to the Debye-Waller effect. As Lead is known to have a very high electron-phonon coupling constant, the Pb lattice is expected to be excited with a timeconstant of less than a picosecond. However, the phonon system is reacting slower than that, with a timeconstant of 3.2 ps.

## Structural Analysis of Ordered Monolayers of the Lander-Type Molecule DBP on Ag(100) via STM and LEED

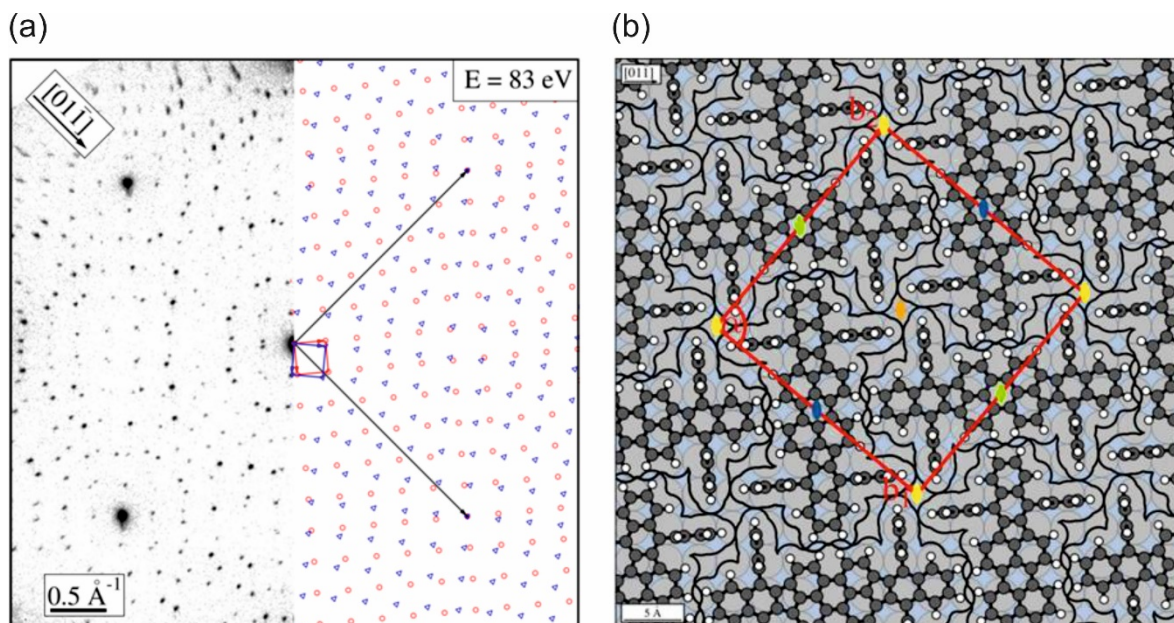
**Beatrice Wolff, Christian Marquardt, Yifei Zhan, Timo Heepenstrick, Robert Harbers, Moritz Sokolowski**

Institut für Physikalische und Theoretische Chemie, Universität Bonn,  
Wegelerstraße 12, 53115 Bonn

We report a combined SPA-LEED and STM investigation on the ordered monolayer structure of the perylene derivate lander-type molecule DBP (dibenzotetraphenylperiflanthene). It consists of a stiff body of dibenzodiindenoperylene and four rotatable phenyl groups serving as “legs”. DBP is a highly fluorescent molecule and has recently been used as an electron donor in organic solar cells [1]. From SPA-LEED images we derive a commensurate structure with a quadratic unit cell of 2.26 nm side length, containing two molecules each. The molecular monolayer displays a p4g symmetry. Adsorbed on the silver(100) surface it can exhibit either a p2 or p4 symmetry, depending on the adsorption site. The LEED pattern shows two symmetry equivalent domains. The molecule forms large islands on the substrate, which can be observed by STM. We discuss possible mechanisms leading to the formation of this structure.

### References

[1] D. Fujishima *et al.*, Solar Energy Mat. and Solar Cells **93**, 1029, (2009)



**Figure 1:** (a) LEED pattern of DBP on the Ag(100) surface with simulation. (b) Possible structural model displaying a p2 symmetry

## Notes

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