O 89: Metal and Semiconductor Substrates: Structure, Epitaxy and Growth

Time: Thursday 15:00–17:45 Location: H8

O 89.1 Thu 15:00 H8

From Unit Cells to Diffraction Patterns: `celltools`, a Python Toolkit for Structural Modeling — •Sebastian Hammer[1] and Bradley J. Siwick[2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Departments of Physics and Chemistry, McGill University, Montreal H3A 0B8, Canada

The coupling of lattice and electronic system crucially determines the properties of modern materials. This interaction is at the heart of many emergent phenomena, such as charge-density wave formation, polaron dynamics, and transient metal-insulator transitions, which have peaked the interest of researchers.

While electronic properties can often be reliably described by quantum chemical methods, capturing structural changes is computationally more demanding. Hence, diffraction experiments are the usual method of choice to investigate structural distortions. However, extracting atomic positions from diffraction data is tedious and not straight forward.

In this contribution, I introduce the python package `celltools`, a versatile tool for constructing and manipulating unit cells as well as simulating their diffraction patterns. Using the case study of excimer formation in the prototypical molecular semiconductor zinc-phthalocyanine investigated with ultra-fast electron diffraction [1], I demonstrate how this tool enables the extraction of momentary atomic position from time-resolved diffraction datasets.

[1] S. Hammer *et al.*, *PNAS* (2024)

O 89.2 Thu 15:15 H8

Automation of data acquisition and measurement evaluation in LEED $I(V)$ — •Florian Dörr[1], Michael Schmid[1], Lutz Hammer[2], Ulrike Diebold[1], and Michele Riva[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Solid State Physics, FAU Erlangen, Germany

We designed a system capable of acquiring and evaluating quantitative low-energy electron diffraction [LEED $I(V)$] data, the Vienna Package for Erlangen LEED (ViPErLEED). The system contains three parts: One part performs data acquisition and is discussed in this contribution. The other two parts focus on the extraction of LEED-$I(V)$ curves from image series [1] and simulation of $I(V)$ spectra for quantitative structure optimization [2].

The data acquisition package consists of open-source hardware for controlling the LEED electronics and software for calibration and the actual measurements. Compared with previous solutions, the package contains functions that improve data quality, such as low-noise measurement of the beam current I_0, automatic calibration of the beam energy, and analysis of the response time of the LEED controller. On the image acquisition side, the software corrects for deficiencies of the camera, such as hot or dead pixels. We will discuss issues that affect the accuracy and duration of LEED-$I(V)$ measurements; this is especially important for sensitive samples that easily degrade.

[1] https://doi.org/10.48550/arXiv.2406.18413
[2] https://doi.org/10.48550/arXiv.2406.18821

O 89.3 Thu 15:30 H8

X-ray reflectivity of μm-samples — •Steffen Tober[1], Wieland Corts[1,2], Steven Leake[3], Toka Matar[1,2], Lisa Randolph[1], Breno Saraiva[4,5], Vedran Vonk[4], Andreas Stierle[4,5], and Hans-Georg Steinrück[1,2] — [1]Forschungszentrum Jülich, Institute for Sustainable Hydrogen Economy (INW), Jülich — [2]RWTH Aachen, Institute of Physical Chemistry, Aachen — [3]ESRF, Grenoble — [4]Deutsches Elektronen-Synchrotron (DESY), Centre for X-Ray and Nanoscience (CXNS), Hamburg — [5]University of Hamburg, Physics Department, Hamburg

X-ray reflectivity (XRR) non-destructively probes electron density profiles of surfaces and interfaces with sub-nm resolution. Large beam footprints in grazing-incidence geometries commonly limit XRR to mm-sized, flat samples because the beam spillover for smaller samples significantly reduces the signal to noise ratio. To probe samples such as individual particles in electrodes or catalysts, a significant reduction of the footprint is needed. As demonstrated for crystal truncation rods [1], the nm-sized X-ray beams of modern synchrotron sources can be used for XRR on μm-sized samples with reduced footprint. We present first proof-of-principle studies comparing XRR of mm- and μm-sized thin-film samples measured with 80 and 400 nm X-ray beams at ESRF ID01 and the necessary optimisation of alignement- and scan procedures [2]. Our results show the general feasibility of nm-beam XRR to be adapted for future *in situ/operando* studies.

[1] J. Stubbs et al., Clays Clay. Miner. 69, 688 (2021)
[2] S. J. Leake et al., J. Synchrotron Rad. 26 571 (2019)

O 89.4 Thu 15:45 H8

How a quartz crystal microbalance reacts to a thermal load — Martina Fellinger[1], Eduardo Pitthan[2], Christian Cupak[1], Friedrich Aumayr[1], Daniel Primetzhofer[2], and •Michael Schmid[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Department of Physics and Astronomy, Uppsala University, Sweden

The most common technique for measuring deposition rates in vacuum is the quartz crystal microbalance (QCM). QCMs are also employed for the determination of sputter yields; further applications are in chemistry and biology. In all these applications, the response of the resonance frequency f to temperature is important. Apart from the crystal's sensitivity to a homogeneous temperature [the $f(T)$ curve], the influence of the thermal stress on the frequency has to be taken into account. In contrast to standard AT-cut crystals, SC-cut (stress-compensated) crystals are insensitive to radial stress. Therefore, SC-cut crystals are used for high-precision measurements or if the power dissipated on the crystal is high (e.g., for sputter yield measurements). Nevertheless, stress effects must be taken into account if the heat source is not exactly centered. The static $f(T)$ response and the effects of local heating, including stress effects, lead to a superposition of a fast response (within $\lesssim 1\,\mathrm{s}$) and a slow frequency change over several minutes; the latter being related to the thermal resistance between the crystal and the crystal holder. Examples of finite-element simulations for a localized heat source will be shown and compared to experimental data of SC-cut crystals irradiated by MeV ions with up to 70 mW power, causing a temperature increase by up to 100 K.

O 89.5 Thu 16:00 H8

Bilayer Formation of Tl on Ag(111): Spatial and Electronic Structural Insights — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Applied Physics, Osaka University, Japan

Ultrathin thallium films on Ag(111) have become a model system for studying the spatial and electronic properties of atomic-layer systems [1-3]. In this study, we focus on investigating the formation of bilayer Tl on Ag(111), leveraging Auger electron spectroscopy, low energy electron diffraction (LEED), and inverse photoemission (IPE) to investigate both spatial and electronic structure. LEED studies indicate that the Tl layers are rotated with respect to the substrate, with the angle of rotation depending on the Tl coverage and deposition temperature. Furthermore, IPE measurements reveal distinct unoccupied electronic states for both the monolayer and the bilayer. With increasing deposition time, the intensity of the monolayer-related state is reduced, while the intensity of the bilayer-related state increases. These results provide insight into the bilayer growth mechanism of Tl on Ag(111) and offer experimental criteria for differentiating between mono- and bilayer.

[1] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)
[2] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[3] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)

O 89.6 Thu 16:15 H8

Capping of terbium silicide nanostructures on Si(111) — •Markus Bachler[1], Milan Kubicki[1], Hüseyin Çelik[2], Sören Selve[3], Martin Franz[1], Michael Lehmann[2], and Mario Dähne[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623, Germany — [3]Zentraleinrichtung Elektronenmikroskopie (ZELMI), Technische Universität Berlin, 10623, Germany

Rare earth silicide films on Si surfaces are of great interest because of their appealing properties, such as extremely low Schottky barrier heights on n-type Si, abrupt interfaces, and the formation of two- and three-dimensional films or one-dimensional nanowires. However, a protective layer is required for further utilisation of these properties, and capping by Si has the further advantage of no lattice mismatch to the substrate and the opportunity to form three-dimensionally stacked nanostructures. For this purpose, rare earth silicides on Si(111) with their very low to no lattice mismatch to Si are very promising for epitaxial capping.

Here we studied capping of thin Tb silicide layers on the Si(111) surface with Si by using scanning tunneling microscopy, cross-sectional high-resolution transmission electron microscopy as well as cross-sectional scanning transmission electron microscopy with energy dispersive X-ray analysis. We observed that overgrowth of the Tb silicide layers with amorphous and crystalline Si leads to intact double layers, demonstrating the stability of the Tb silicide layer upon capping.

O 89.7 Thu 16:30 H8

Exploring surface properties of hexagonal Si and Ge — •Martin Keller[1], Abderrezak Belabbes[1,2], Jürgen Furthmüller[1], Friedhelm Bechstedt[1], and Silvana Botti[1,3] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Sultan Qaboos University, Muscat, Oman — [3]Ruhr Universität Bochum, Germany

We present ab initio calculations, using density functional theory in a slab geometry, that explore structural and electronic properties of the surfaces of hexagonal silicon and germanium, which are novel materials for active optoelectronic applications. We study the relaxed 1×1 a, m, c and r-plane facets, who's surface energies allow the creation of Wulff constructions of Si and Ge nanocrystals and wires. Our focus lies on understanding surface stability and its implications on material and device design, as well as the effects of the relaxation on the electronic properties. The comparison with experimental findings offers practical insights for substrate selection for thin film growth and the construction of heterostructures.

O 89.8 Thu 16:45 H8

Strong electron doping of single-layer MoS_2 on an oxidized contact — •Marco Bianchi[1,2], Charlotte Sanders[3], Davide Curcio[4], Daniel Lizzit[5], Paolo Lacovig[1], Ezequiel Tosi[6], Jill Miwa[2], Silvano Lizzit[1], and Philip Hofmann[2] — [1]Elettra Sincrotrone Trieste S.C.p.A., Trieste, IT — [2]Dep. of Physics and Astronomy, iNANO, Aarhus University, DK. — [3]Artemis Program, UK Central Laser Facility, Harwell, STFC, UK — [4]IOM, Consiglio Nazionale della Ricerca, Trieste, IT — [5]DPIA - University of Udine, IT — [6]Instituto de Ciencia de Materiales de Madrid (ICMM - CSIC), ES

One of the major obstacles for the use of two-dimensional semiconductors in devices continues to be the high contact resistance to metallic conductors and the associated losses. Promising results have recently been obtained by using group V semimetals as contact materials. The obtained low contact resistance was explained partly by the a degenerate doping of the two-dimensional semiconductor. Here we study the band alignment and structure of such a system, a single-layer of MoS_2 on Au(111) with an intercalated layer of Bi. We investigate the electronic structure and growth by angle-resolved photoemission spectroscopy, X-ray photoemission spectroscopy, low energy electron diffraction and scanning tunneling microscopy. Our results show no evidence for an occupation of the MoS_2 conduction band when the material is brought into close contact with Bi. Surprisingly, however, a subsequent oxidation of the intercalated Bi gives rise to an extremely strong electron doping of the conduction band with a carrier density on the order of 10^{13} cm^{-2}.

O 89.9 Thu 17:00 H8

Growth of two-dimensional Ta-S structures from TaS_3 nuclei to TaS islands — •Catherine Grover[1], Alice Bremerich[1], Kai Mehlich[1], Abdus Samad[2], Udo Schwingenschlögl[2], Carsten Busse[1], and Thais Chagas[1] — [1]Department Physik, Universität Siegen, D-57072 Siegen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900 Thuwal, Saudi Arabia

Transition metal dichalcogenides (TMDCs) are emerging as promising 2D materials, known for their unique physical and electronic properties. Despite the rapid growth of research in this field, the exact mechanisms governing their growth remain largely speculative, especially when compared to more well-understood systems, such as metal-on-metal growth.

In this study, we employ Scanning Tunneling Microscopy (STM) to investigate the growth process of ultrathin tantalum sulfide (Ta-S) phases. We observe the evolution from embedded TaS_3 nuclei to Ta_3S_6 islands, and ultimately to TaS islands. These findings provide new insights into the growth dynamics of Ta-S phases, revealing the underlying processes.

Furthermore, these structural observations are supported by Density Functional Theory (DFT) calculations, which compare the energies of various structures, offering additional validation of the experimental results.

O 89.10 Thu 17:15 H8

Ab initio surface phase diagram of $(Al_xGa_yIn_{1-x-y})_2O_3$ — •Qaem Hassanzada[1], Yuanyuan Zhou[1,2], and Matthias Scheffler[1] — [1]The Fritz Haber institute, Berlin, Germany — [2]The Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Group III sesquioxides with ultra-wide bandgaps are the most promising candidates for high-power electronics. Numerous efforts have been made to grow group-III sesquioxides, however, the fundamental understanding of growth process is still shallow. The prerequisite to understand growth process is detailed information about the surface geometry and stoichiometry under growth conditions. This can be provided in surface phase diagrams. In this study, we explore the surface phase diagram of Group III sesquioxides, $(Al_xGa_yIn_{1-x-y})_2O_3$, for the entire compositional range, using ab initio atomistic thermodynamics [1, 2] and the sure-independence screening and sparsifying operator (SISSO) [3] machine learning methods. We predict the most probable phases under the corresponding growth conditions. For instance, in the Ga-rich region, we predict the formation of a Ga monolayer, which may be related to the experimental hypothesis of Ga adlayer formation at a lower O/Ga ratio [4] reminiscent of the phenomena in GaN.

[1] Scheffler, M. Studies in Surface Science and Catalysis, Vol. 40; Elsevier: 1988, pp 115−122. [2] Reuter, K.; Scheffler, M. Phys. Rev. B 2001, 65, 035406. [3] Ouyang, R. et al. M. Phys. Rev. Mater. 2018, 2, 083802. [4] Chou, T. et al. AIP Advances 2021, 11, 115323.

O 89.11 Thu 17:30 H8

Ultrathin NiO(100) films on Ag(100): Pitfalls in understanding growth using intensity-voltage low-energy electron diffraction — •Jan Lachnitt[1], Shuvankar Das[2], Krishnakumar S. R. Menon[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Germany — [2]Surface Physics & Material Science Division, Saha Institute of Nuclear Physics, Kolkata, India

Ultrathin NiO films have prospective applications in heterogeneous catalysis, microelectronics, and spintronics and are thus an object of active research. In model systems, the Ag(100) surface is frequently used as support for these films, as its cubic lattice parameter is only 2.2% smaller than that of NiO, enabling pseudomorphic growth for very small thicknesses. Interestingly, the early-stage growth of NiO films on Ag(100) turns out to be complex compared to other simple oxide systems, such as MgO/Ag(100). We have grown pseudomorphic NiO(100) films of well-defined average thickness in steps of 0.5 monolayer (ML), up to 3 MLs, and studied them with intensity-voltage low-energy electron diffraction (IV-LEED). We have also employed density-functional theory (DFT) calculations to gain additional insights. Our IV-LEED results indicate a deviation from layer-by-layer growth, expected to take place from 2 MLs onwards [1], and the detailed analysis of the oxide-metal system has turned out to be tricky. We discuss the pitfalls and limitations of common IV-LEED procedures and compare the results with our DFT calculations and existing literature.

[1] J. Wollschläger et al., Thin Solid Films 400 (2001) 1.