O 112: Development of Novel Methods I

Time: Thursday 15:00–17:30 Location: WIL C107

Invited Talk O 112.1 Thu 15:00 WIL C107

Positron Beams for Elemental and Structure Analysis of Surfaces — •Christoph Hugenschmidt — MLZ and Physics Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

With the advent of bright low-energy positron beams novel analysis tools have been developed exploiting the unique properties of positron matter interaction such as repulsive crystal potential or positron trapping in surface states [1]. Positron annihilation is established for defect spectroscopy and the characterization of the free volume in amorphous matter. By applying a slow positron beam, however, defects near the surface can be specifically addressed, e.g. for the determination of the O vacancy concentration in YBa2Cu3O7-x [2]. The positron counterparts of reflection high-energy electron diffraction (RHEED) and electron induced Auger-electron spectroscopy (AES) intrinsically exhibit superior surface sensitivity. In contrast to electrons, positrons show total reflection for small glancing angles. It was demonstrated that with reflection high-energy positron diffraction the structure of the topmost and the immediate subsurface atomic layer of surfaces can be revealed with outstanding accuracy. The main advantages of positron annihilation induced AES are the missing secondary electron background and its topmost layer sensitivity for elemental analysis, e.g. for the in situ observation of the Ni adatom migration from the Pd surface into the bulk [3]. [1] C. H.; Surf. Sci. Reports 71 (2016) 547 [2] M. Reiner et. al.; Phys. Rev. B 97 (2018) 144503 [3] S. Zimnik et. al.; Surf. Sci. 664 (2017) 61

O 112.2 Thu 15:30 WIL C107

X-Ray Absorption Spectroscopy at Free-Electron Lasers using a Split-Beam Referencing Scheme — •Robin Y. Engel[1,3], Günter Brenner[1], Siarhei Dziarzhytski[1], Piter S. Miedema[1], Jan Schunck[1,3], Florian Döring[2], Benedikt Rösner[2], Christian David[2], and Martin Beye[1] — [1]Deutsches Elektronen Synchrotron DESY, Germany — [2]Paul Scherrer Institut, Switzerland — [3]Universität Hamburg, Germany

Any absorption spectroscopy is based on the exact measurement of the ratio between incident and transmitted intensity. If the used light-source provides a constant incident intensity, measuring only the transmitted light can be sufficient. In order to measure X-ray Absorption Spectra (XAS) with a time-resolution on the fs-scale, X-ray sources with high brilliance and short pulse duration are required. Modern Free Electron Lasers (FEL) deliver such pulses, but most exhibit a strongly fluctuating spectral content, so that an exact measurement of both incident and transmitted intensities becomes necessary. This can be achieved using a diffraction grating in transmission that splits the FEL beam into two identical copies (+/- 1. diffraction order) which are used as probe- and reference-beams. For ideal comparability, both beams are measured on the same CCD-detector after one of them has interacted with the sample. This concept was implemented at the Free Electron LASer in Hamburg (FLASH) both in transmission and reflection geometries. X-ray absorption spectra can be recorded either in monochromatic mode, or by directly normalizing two copies of an energy-dispersed beam on the same CCD.

O 112.3 Thu 15:45 WIL C107

Two-dimensional spin detection with high-resolution laser ARPES based on hemispherical analyzer and exchange scattering spin detector — •Tristan Heider, Claus M. Schneider, and Lukasz Plucinski — FZ Jülich PGI-6, Jülich, Germany

Two existing approaches for measuring 2D spin maps in angle-resolved photoemission are single k-point detectors behind the hemispherical analyzer [1], and 2D spin detectors in combination with momentum microscopes, either with hemispherical [2] or time-of-flight energy filtering (other related concepts exist). Here we describe the setup of the first type based on the *A*1 hemispherical analyzer with the lens deflection system (MBS AB) with the *Ferrum* spin detector (Focus GmbH) mounted on a 90-deg deflector. The point-by-point spin scanning is efficient when using the 6eV *cw* laser excitation (LEOS Solutions), and a typical 50 × 50 pixel 2D spin map can be collected within 10-20 min. The unique advantages are the access to both in-plane and out-of-plane spin components using *Ferrum*, the negligible instrumental asymmetries, and the access to the energy resolution down to 5 meV in spin. We will discuss several applications, including the high resolution spin-integrated laser-ARPES from Fe-based superconductor, and spin-resolved in-plane and out-of-plane 2D spin-texture from the Bi_2Se_3-family material. The challenges in data collection of our large 3D ARPES maps will be discussed in a separate talk [3].

[1] L. Plucinski et al. J. Electron Spectroscopy Rel. Phen. 181, 215 (2010) [2] C. Tusche et al., Ultramicroscopy 159, 520 (2015) [3] L. Plucinski et al., this conference

O 112.4 Thu 16:00 WIL C107

The TensErLEED Management Package: A new environment for analysis and calculation of IV-LEED data — •Florian Kraushofer[1], Michael Schmid[1], Ulrike Diebold[1], Lutz Hammer[2], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]FAU Erlangen-Nürnberg, Erlangen, Germany

Low Energy Electron Diffraction (LEED) is a structure sensitive technique commonly available in most surface science laboratories. Beyond the usual application as a tool to determine periodicity and degree of order of a surface phase, quantitative analysis of the modulation of beam intensities as a function of voltage (IV-LEED) allows direct comparison to theoretically predicted structural models. This, however, requires complex full-dynamical intensity calculations as well as a time-consuming optimization of structural parameters minimizing the deviation between experimental and calculated $I(V)$ curves. The Erlangen program package TensErLEED [1] readily performs this task, but its required user input is almost prohibitively complex.
We show that for most cases, the necessary TensErLEED input can be generated automatically by combining a handful of user parameters, a set a default values, and a structure file in a standard format. Based on this, we introduce a new package that greatly simplifies the use of TensErLEED and substantially reduces the amount of work and potential for errors, even for experienced users. The package is completed by a versatile utility for extracting experimental $I(V)$ spectra from a LEED video or a stack of LEED images.
[1] V. Blum, K. Heinz, Comput. Phys. Commun., 2001. 134(3)

O 112.5 Thu 16:15 WIL C107

Photoelectron Momentum Imaging Using a Combination of Single Hemispherical Analyzer and Time-of-Flight Recording — •Katerina Medjanik, Sergey Babenkov, Dmitry Vasilyev, Hans-Joachim Elmers, and Gerd Schönhense — JGU, Institut für Physik, Mainz, Germany

Extensive work of Tusche et al. [1] uncovered principal advantages of the "non-inverted" operation of a double-hemispherical analyser, a concept that can be simplified to a large single hemispherical dispersive analyser (HDA). We implemented an additional time-of-flight (ToF) section behind the HDA as "booster" improving resolution. The time spread of the electrons passing the HDA is detrimental in standard operation [2] but is strictly deterministic in our instrument, because the momentum image is encoded as angular pattern in the analyzer. First data taken with laboratory sources show that the time spread (1-2 ns at typical settings) varies linearly with coordinate ky (dispersive direction) but does not affect kx. Combining the flexibility of the HDA with the advantage of 3D ToF-recording, the hybrid instrument increases detection efficiency by 1-2 orders of magnitude. It does not require special filling patterns of Synchrotron- and FEL-sources and will be most relevant for high-resolution and spin-resolved work in the soft- and hard-X-ray range, where ToF-recording has proven superior [3].

[1] Tusche et al., Ultramicr. 206, 112815 (2019); [2] Sise & Zouros, J. Spectroscopy 153513 (2015); [3] Medjanik et al., J. Synchr. Rad. 26, 1996 (2019).

O 112.6 Thu 16:30 WIL C107

Adsorption controlled permeation as a new approach in surface science — •Petr Dementyev — Bielefeld University, Bielefeld 33615, Germany

Molecular adsorption on solids and interfacial diffusion are of paramount importance in heterogeneous chemistry and membrane separation. Recently, two-dimensional (2D) materials have been employed as ultrathin windows for probing related surface phenomena. In particular, X-ray photoelectron spectroscopy with radiation transparent

films has been significantly advanced to be applied under realistic reaction conditions. Herein, we introduce another methodology based on the ultimate thickness of free-standing 2D membranes - Adsorption Controlled Permeation (ACP). As there is no much internal volume, mass transfer across porous planar nanomaterials is expected to be dominated by entrance kinetics. We demonstrate experimentally that studying transport rates in 2D layers yields unprecedented information on physicochemical processes ranging from condensation to solvation. The ACP measurements are carried out in an originally designed vacuum system with a mass-spectrometric detector. Vapor permeation studies with carbon nanomembranes (CNMs) reveal that adsorbed species are able to promote transmembrane diffusion of non-condensable gases. Furthermore, concentration-induced disruption of single-file water was discovered to take place in narrow nanochannels.

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O 112.7 Thu 16:45 WIL C107

Optimization of a UHV-compatible electrochemical flow cell combined with IRAS and DEMS for single crystal experiments — •Claus Kovacs, Jiri Pavelec, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson — Institute of Applied Physics, Vienna University of Technology, Austria

Electrochemical reactions involving metal-oxide catalysts are increasingly important in energy conversion technologies, but the mechanisms involved remain shrouded in mystery. Electrochemical surface science is relatively well established, but studies involving metal-oxide single crystals remain rare, and best practices for UHV-to-electrolyte transfer are still being established. Here, we will discuss the development of a UHV-compatible electrochemical flow cell, which is to be combined with in-situ differential electrochemical mass spectroscopy (DEMS) and infrared reflection absorption spectroscopy (IRAS) measurements. Crucially, the transfer must be made without exposure to air. To speed up the design process and optimize cell performance, we have performed numerical simulations utilizing the program COMSOL Multiphysics®. In particular, the simulations allow us to optimize the thickness of the flow cell, which has a major impact on IRAS and the electrochemical cell performance. Further, the residence time in the cell is also optimized to improve DEMS detection. The simulations focus on mass transport through the cell, as well as the reaction at the catalytic interface. Finally, charge transport is studied to optimize the position and shape of the counter and reference electrodes.

O 112.8 Thu 17:00 WIL C107

shear flow-driven dewetting for wrinkle-free transfer of centimeter-scale ultrathin alumina membrane onto arbitrary substrates — •Huanming Zhang, Min Zhou, Rui Xu, and Yong Lei — Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau

The transfer of ultrathin membrane (UTM) onto arbitrary substrates is important in different practical fields. The polymer-supported transfer of UTM keeps the structure of membrane intact, but suffers from organic residual. Wet transfer is applicable to the UTM without a polymer support, where the liquid surface serves as an underlying support. However, conventional wet transfer methods inevitably induce wrinkle defects as a result of the large contact angle of the trapped droplet between UTM and substrate. To solve this problem, the target substrates always need either hydrophilic treatments or organic liquid wetting. However, they are not applicable to all the substrates. Here we demonstrate a shear flow-driven dewetting method to transfer centimeter-scale membrane onto arbitrary substrates without wrinkle. Compared with hydrophilic treatments or organic liquid wetting, this method is fast, simple, cheap, convenient and safe. Taking widely-used ultrathin anodic aluminum oxide membrane (UTAM) as an example, we investigate the microscale details of these macroscale wrinkles and successfully demonstrate the application of large-area wrinkle-free UTAM to defect-free ordered nanostructure arrays fabrication. Corresponding superiority over the defective counterpart is further studied in optical sensing.

O 112.9 Thu 17:15 WIL C107

Preparative mass spectrometry using electrospray controlled-ion-beam-deposition device — •Andreas Walz, Karolina Stoiber, Wei Ran, Annette Hüttig, Joachim Reichert, Hartmut Schlichting, and Johannes V. Barth — Physics Department E20, Technical University of Munich, Germany

Designing novel nanostructures of organic and anorganic compounds requires precise and controlled growth of atomically clean films of clusters or molecules on well-defined surfaces. Our home-build Electrospray Controlled Ion Beam Deposition device (ES-CIBD) opens access to the large, reactive and thermolabile species including biomolecules like proteins or DNA which had been excluded form investigation with standard deposition devices. The implemented Quadrupole Mass Spectrometer (QMS) allows for the characterization of the molecules as well as their purification prior to deposition. It is operated in a digital technique, allowing for very high m/z ratios and adaption of the resolution thereto. The innovative Radio Frequency (RF) controlled ion guides preserve the beam intensity of up to 1nA through the subsequent vacuum chambers from ambient conditions to ultrahigh vacuum (UHV). This allows for precise, short-time depositions, soft-landing conditions with 1-2 eV kinetic energy may be adjusted as well as reactive-landing conditions with some 100 eV. Simulations with SIMION assisted the design. Scanning tunneling microscopy (STM) investigations of large plasmid DNA molecules (1,7 MDa) and N-doped graphene nanoribbons proof quality and versatility of the depositions performed with the instrument.