O 53: Nanostructures at Surfaces: Other Aspects

Time: Tuesday 18:30–20:30 Location: P1C

O 53.1 Tue 18:30 P1C

Modelling of surface properties of beryllium-tungsten alloys — •Alexander Kaiser[1], Ivan Sukuba[1,2], Lei Chen[1], Jan Urban[2], and Michael Probst[1] — [1]Institute for Ion Physics and Applied Physics, University of Innsbruck, Innsbruck, Austria — [2]Technikerstraße

The high melting of tungsten and its resilience against physical sputtering make it a favorable material for plasma facing components with high heat loads. Beryllium is a very light, low-Z material and a neutron multiplier and also has other favorable properties such as a low tritium solubility. In the ITER thermonuclear fusion experiment, beryllium will be used for the first wall and tungsten for the divertor. Sputtering, transport, and deposition of these materials can lead to alloy formation in the device. With quantum chemical methods, we try to shed some light on the stability and the reactivity of Be, W, and selected alloys of Be and W, including their sputtering properties.

O 53.2 Tue 18:30 P1C

Surface Modifications of Various Ionic Fluoride Single Crystals by Slow Highly Charged Ions — •Ayman S. El-Said[1], Richard A. Wilhelm[2,3], René Heller[2], Friedrich Aumayr[3], and Stefan Facsko[2] — [1]Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Institute of Applied Physics, TU Wien, 1040 Vienna, Austria

The creation of surface nanostructures is of high importance for today's nanoelectonics and nanophotonics applications. Slow highly charged ions (HCI)have demonstrated their uniqueness and effectiveness in the formation and control of nanostructures in various materials. Here, we focus on the surface modifications induced by HCI in alkali (LiF) and alkaline-earth (CaF2 and BaF2) fluoride single crystals. The surfaces were irradiated with HCI of different charge states and kinetic energies. In case of CaF2 and BaF2, only one type of nanostructures (hillocks) was observed after surpassing certain potential energy thresholds for the incident HCI. For LiF, HCI were able to create three types (pits, calderas, and hillocks) of nanostructures by varying the impinging ions' charge states, or microscopically the locally deposited potential energy. The results are discussed in terms of defect-mediated desorption and thermal spike models.

O 53.3 Tue 18:30 P1C

Controlling charge fluctuations of a few donor system — •Ole Bunjes, Philipp Kloth, Judith von der Haar, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Combining a low temperature Scanning Tunneling Microscope with optical excitation, we have investigated temporal charge fluctuations within the tip induced space charge region. Our studies on the (110) surface of n-doped GaAs have shown that the system can be driven into different non-equilibrium states due to optically induced minority charge carriers [1]. Analysis of the noise characteristic of the tunnel current reveals the influence of photo-generated holes on dynamical charging processes. The presence of these free charges allows us to change and control the noise characteristic of the system. The noise level depends on the laser intensity as well as the tunnel current, controlled by the tip-sample-distance. Most surprisingly, the overall noise can even be reduced compared to the non-illuminated system. We attribute the optically induced modification of the noise characteristic to temporal charging and discharging of dopant atoms within the space charge region [2]. We acknowledge the financial support by the SFB1073 C04. [1] P. Kloth et al., Nat. Commun. 7, 10108 (2016) [2] K. Teichmann et al., Nano Lett. 11, 3538-3542 (2011)

O 53.4 Tue 18:30 P1C

Controlling charge dynamics in a space charge region under optical excitation — •Judith von der Haar, Philipp Kloth, Ole Bunjes, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

By combining laser excitation and Scanning Tunneling Microscopy we have investigated the charge dynamics of a few donor system at the n-doped GaAs(110) surface. When a STM-tip is positioned close to the GaAs a SCR is induced inside the sample. In equilibrium it is screened by ionized donors at the surface. We force the system out of equilibrium by illuminating the sample and generating free charge carriers. The photo-generated holes can be addressed by tunneling electrons, leading to an additional transport channel. Using the tunnel current as a control parameter we are able to actively change the hole concentration at the surface [1]. The temporal evolution of the photo-generated holes was studied for different laser intensities, tunnel currents and bias voltages using pulsed optical excitation with nanosecond time resolution [2]. This gives access to the screening dynamics of the tip-induced potential. Furthermore, we have measured the charging and discharging processes of single donors. Atomically resolved data proof that the relaxation time depends on the relative depth of the donors to the surface. This work was supported by the DFG via the SFB1073 C04. [1] P. Kloth et al., Nat. Commun. 7, 10108 (2016) [2] P. Kloth et al. A versatile implementation of pulsed optical excitation in Scanning Tunneling Mircroscopy. Rev. Sci. Instr. (acc. 2016)

O 53.5 Tue 18:30 P1C

Neon ion beam induced pattern formation on amorphous carbon surfaces — •Omar Bobes, Hans Hofsäss, and Kun Zhang — II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

We investigate the ripple pattern formation on amorphous carbon surfaces at room temperature during low energy Ne ion irradiation as a function of ion incidence angle. Monte Carlo simulations of the curvature coefficients applied to the Bradley-Harper and Cater-Vishnyakov models, including the recent extensions by Harrison-Bradley and Hofsäss and taking into account the incorporation of the ions into the film predict that pattern formation on amorphous carbon should be possible for low energy Ne ions from 250 eV up to 5 keV. Moreover, simulations are able to explain the absence of pattern formation in certain cases. Our experimental results are compared with prediction using current linear theoretical models and applying the crater function formalism as well as Monte Carlo simulations to calculate curvature coefficients using SDTrimSP program.

O 53.6 Tue 18:30 P1C

Treatments of high-density polyethylene (HDPE) with atomic hydrogen - a surface study — •Torben Schlebrowski, Christian B. Fischer, and Stefan Wehner — Department of Physics, University of Koblenz-Landau, 56070 Koblenz, Germany

The deposition of diamond-like carbon (DLC) films on materials like polymers is a well-established method for substrate surface modification and its refinement. The interaction of atomic hydrogen with polymers in contrast is not well studied, although it is part of the most techniques used for DLC depositions. For a complete description of the carbon deposition process it is inescapable to study this aspect, since the hydrogen is supposed to change and modify the polymeric substrate surface by impinging. Measurements by in situ thermal desorption spectroscopy (TDS) during hydrogen treatment are performed to analyze process products and by atomic force microscopy (AFM) surface changes due to the hydrogen processing are revealed. The contribution shows first results for the interaction of atomic hydrogen with common polymers as HDPE.

O 53.7 Tue 18:30 P1C

Investigating the switching behaviour of a Tetraphenylmethane-Derivative on Au(111) with STM — •Timo Frauhammer[1,2], Lukas Gerhard[2], Kevin Edelmann[2], Marcin Lindner[2], Michal Valasek[2], Marcel Mayor[2], and Wulf Wulfhekel[1,2] — [1]Physikalisches Insitut, Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe, Germany

The adsorption and switching behaviour of a Tetraphenylmethane-derivative adsorbed on Au(111) have been studied using scanning tunneling microscopy (STM) at 5.3 K. This derivative consists of a Tetraphenylmethane-core where the four Hydrogen atoms in para-position with respect to the central sp3-Carbon atom are substituted by three Thioacetate-groups and one Triflate-group. The molecules have been deposited on Au(111) from a Dichloromethane solution by

using a spray technique. The tip of the STM induces a characteristic switching behaviour between two metastable states. Moreover, Random Telegraph Noise (RTN) can be observed at certain tunneling parameters. The functional dependence of this RTN on bias voltage and tip-sample distance indicates that the switching is induced by the electrical field in the tunnel junction.

O 53.8 Tue 18:30 P1C

Universal readers based on hydrogen bonding or π-π stacking for identification of DNA nucleotides in electron tunnel junctions — •Suman Sen[1], JongOne Im[2], Peiming Zhang[2], and Stuart Lindsay[2] — [1]Max Planck Institute, Stuttgart, Germany — [2]Arizona State University, Tempe, USA

A universal reader molecule, which recognizes all the naturally occurring nucleobases in a tunnel junction, is required for sequencing DNA by a recognition tunneling (RT) technique. We have designed a series of heterocyclic carboxamides based on hydrogen bonding and a large-sized pyrene ring based on a π-π stacking interaction as reader candidates. RT measurements were carried out in a scanning tunnel microscope. All of these molecules generated electrical signals with DNA nucleotides in tunneling junctions under physiological conditions. Using a support vector machine as a tool for data analysis, we found that these candidates distinguished among naturally occurring DNA nucleotides with the accuracy of pyrene > azole carboxamides. In addition, the pyrene reader operated efficiently in a larger tunnel junction. However, the azole carboxamide could read abasic monophosphate, a product from spontaneous base hydrolysis or an intermediate of base excision repair. Thus, we envision that sequencing DNA using both π-π stacking and hydrogen-bonding-based universal readers in parallel should generate more comprehensive genome sequences than sequencing based on either reader molecule alone.

O 53.9 Tue 18:30 P1C

Hyperuniformisation by Lloyd's algorithm for Centroidal Voronoi diagrams — •Jakov Lovrić[1,2], Philipp Schoenhoefer[3,4], Sebastian Kapfer[3], Fabian Schaller[3], Michael Klatt[5], Bruce Gardiner[4], Ana-Sunčana Smith[1,2], and Gerd Schröder-Turk[4] — [1]Institute Ruđer Bošković, Division of Physical Chemistry, Group for Computational Biosciencies, Zagreb, Croatia — [2]Institute for Theoretical Physics, PULS Group and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Germany — [3]Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [4]School of Engineering and Information Technology, Murdoch University, Western Australia 6150, Australia — [5]Karlsruhe Institute of Technology (KIT), Institute of Stochastics, Karlsruhe, Germany

We study an application of centroidal Voronoi diagrams and Lloyds algorithm. The simple idea is that the evolution of points under Lloyd's algorithm leads to more uniform structures, in a loose sense. We investigated, and found an initial positive result, that Lloyd's algorithm can be used to achieve hyper-uniform structures when starting from several types of disordered point patterns. We havn't found a point pattern where Lloyd's algorithm does not lead to a hyper-uniform structure. An important question is whether Lloyd's algorithm induces crystalisation of the point configuration; one may have thought this possible, given that the body-centered cubic lattice is considered the configuration with lowest energy w.r.t. the functional used in Lloyd's algorithm.

O 53.10 Tue 18:30 P1C

Biopolymers in Vacuum and at Surfaces — •Stephan Rauschenbach[1], Sabine Abb[1], Elise Duquesne[1], Christian Schön[1], Ludger Harnau[1], Duy Le[2], Talat Rahman[2], and Klaus Kern[1] — [1]Max Planck Institute for Solid State Res., Stuttgart, Germany — [2]Univ. of Central Florida, Tampa FL, USA

Proteins, DNA, and sugars are the main classes of biopolymers. Each, with its unique properties, is essential for living organisms. Thus their thorough characterization is essential to improve our understanding of the complex molecular interactions underlying to the supreme functionality. With soft-landing electrospray ion beam deposition[1], we are able to control the transfer of said classes of polymers onto surfaces in vacuum such that high resolution imaging by scanning tunneling microscopy (STM) can reveal structural details at the submolecular level. This enables unprecedented insights, such as detection of saccharide subunits, sequence controlled assembly and folding of peptides, controlled formation of peptide-metal complexes, or conformation control of proteins. With this work we open routes to new materials based on complex, specific, molecular interaction and enable high resolution structural analysis of individual biopolymers.

[1] S. Rauschenbach et al. **Annu. Rev. Anal. Chem.** 9, 16.1-16.26 (2016)

O 53.11 Tue 18:30 P1C

Simulation of high energy XPD-patterns — •Robert Rauter, Christopher Kohlmann, Tobias Lühr, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Germany, Otto-Hahn-Str. 4, 44221 Dortmund

Photoelectron diffraction (XPD) is a powerful tool to examine surface and interlayer structures of solids. In order to extract the structural information from the experimental data, simulated XPD patterns are compared to experimental XPD patterns. For determining the correct structure a multiplicity of different surface and interface layer structures must be considered within the simulation.

The XPD pattern simulation is performed by the EDAC (Electron Diffraction in Atomic Clusters) package [1]. Reducing the quantity of simulations is achieved by utilizing a genetic algorithm [2]. We report on the improvement of convergence by applying the genetic algorithm in comparison to a deterministic approach.

[1]F.J. Garcia de Abajo, M.A. Van Hove and C.S. Fadley, Phys. Rev. B **63**, 075404 (2001).
[2]Pancotti, A. et al., J. Appl. Phys. **106**, 34104 (2009).

O 53.12 Tue 18:30 P1C

Considering the Convergent Beam in a Quantitative LEED Analysis — •Tilman Kisslinger, Pascal Ferstl, M. Alexander Schneider, and Lutz Hammer — Lehrstuhl für Festkörperphysik, Universität Erlangen–Nürnberg, D–91058 Erlangen, Germany

In a conventional LEED experiment the primary electron beam is not parallel, but slightly convergent (opening angle typically $2 \times 0.6°$), in order to focus the beam on the screen. Thus, experimental LEED intensity spectra are in fact a superposition of spectra belonging to all angles within that cone of incidence, therefore, model calculations performed for the central cone angle are just an approximation of the experimental situation.

For nominally normal incidence of the primary beam, which is the common experimental alignment, as it preserves a maximum of symmetry elements of the surface, we performed a pseudo–experiment, in which for a Rh(100)–(2×2)–O surface intensity spectra were calculated for various angles within a cone of $\Theta_{max} = 0.75°$, weighted according to their corresponding solid angle and averaged. A comparison with the set of spectra calculated for normal incidence yields a R_P of 0.036. It is further shown that using an average cone angle $\Theta_{av} = \Theta_{max}/\sqrt{2}$ instead fits the pseudo-experiment with high accuracy ($R_P = 0.0003$). Fitting the (average) angle of incidence for real experimental data of various and structurally very different systems taken nominally at normal incidence always led to an improvement of the R-factor by about 0.02 - 0.03. Consistently, all fits result in the same value for Θ_{av}, because it is solely determined by the experimental geometry.