O 97: Nanostructure at Surfaces: Structures and Properties

Time: Friday 10:30–12:45 Location: MA 005

O 97.1 Fri 10:30 MA 005

Thin diamond-like carbon (DLC) coatings on bio plastic films of polyhydroxybutyrate (PHB) — •Christian B. Fischer and Stefan Wehner — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

Bio generated and biodegradable polymers represent a promising alternative for conventional petroleum-based plastics. These bio plastics are ideal for packaging in food industry, agricultural usage or in the medical field. In many cases parent plastic material suits mechanical requirements but exhibits poor surface features, leading to bacterial adhesion, for instance. This can be avoided by appropriate surface modifications. One frequently used technique is the coating of parent material with thin films of diamond-like carbon (DLC) via PECVD. The surface morphologies of a 50 μm thick foil of polyhydroxybutyrate (PHB) coated with two different DLC-types of various thicknesses are examined by SEM and AFM. The r-type is sp3-enriched which results in a more robust layer, and the f-DLC is sp2-enriched, making it more flexible. Layers of r-type up to around 450 nm are intact, further deposition results in cracking and exfoliation of the DLC coating due to increasing internal stress. Furthermore, the effect of an improved understanding of hard DLC and soft PHB material is part of the present work.

O 97.2 Fri 10:45 MA 005

novel structures and phenomena in ultrathin films — •rajib batabyal and bhupendra nath dev — indian association for the cultivation of science, kolkata, india

Nanostructures and thin films on well-defined substrate surfaces, their stability and exploration of new physical phenomena are important aspects not only for the development of future nanoscale devices but also for the advancement of basic physics research.

Here we discuss two major aspects of Ag ultrathin films on Si(111)-7x7 surfaces. In the first section, we demonstrate a new phenomenon related to the electronic transport in 2-D to 3-D crossover. By STS measurement we show the dependence of the negative differential resistance (NDR) with film thickness for one-atomic layer to five-atomic layer thick films. The dependence of the onset voltage at which NDR sets in, is shown as a function of ultrathin film thickness. These results are explained via density functional theory (DFT) calculations. In the other section, we report on a novel mechanism in electric filed induced atomic migration and formation of one-atom thick fractal nanostructures. Application of a voltage pulse at an edge of a flat-top Ag island results in migration of Ag atoms from edge to the top of the island and aggregation to form a precisely one-atom thick fractal Ag layer. Diffusion limited aggregation (DLA) appears to be responsible for the formation of fractal nanostructures. We have also determined various fractal dimensions and corelated them to describe the morphology of fractal clusters.

O 97.3 Fri 11:00 MA 005

Spin-resolved photoelectron spectroscopy of chiral nanostructures — •Daniel Nürenberg[1], Andrew Mark[2], Matthias Kettner[1], Benjamin Göhler[1], Peer Fischer[2], and Helmut Zacharias[1] — [1]Westfälische Wilhelms-Universität, Münster, Germany — [2]Max-Plank-Institut für Intelligente Systeme, Stuttgart, Germany

Helical molecules on surfaces have been shown to affect the spin polarization of photoelectrons excited from the substrate [1]. Further investigation demands new materials, showing similar effects, which offer more degrees of freedom in designing helical potentials than are possible with molecules. Helical nanostructures are a candidate for this. They can be grown on wafer scale size by glancing angle vapor deposition (GLAD) on a turning silicon wafer seeded with Au nanodots. The nanohelices have lengths of around 100 nm, a pitch of approximately 50 nm and show a circular dichroism at visible wavelengths [2]. We present spin- and polarization-resolved photoelectron studies of such nanostructures made of noble metal and noble metal alloys.

[1] Göhler, B.; Hamelbeck, V.; Markus, T.Z.; Kettner, M.; Hanne, G. F.; Vager, Z.; Naaman, R. and Zacharias, Science, 331, 894-897(2011)

[2] Mark, A.G.; Gibbs, J.G.; Lee, T. and Fischer, P., Nat. Mater.,12, 802-807(2013)

O 97.4 Fri 11:15 MA 005

Mechanical properties of surfaces at the nanoscale — •Jörg Buchwald[1] and Stefan G. Mayr[1,2,3] — [1]Leibniz Institute of Surface Modification, Permoserstr. 15, 04318 Leipzig, Germany — [2]Faculty of Physics and Earth Sciences, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [3]Translational Center for Regenerative Medicine (TRM)Leipzig, Philipp-Rosenthal-Str. 55, 04103 Leipzig, Germany

New experimental techniques like contact resonance atomic force microscopy (CR-AFM) allow for non-destructive testing mechanical properties with nanometer resolution. Mechanical properties of surfaces or nanostructures deviate from bulk material due to surface stresses as well as local relaxations. In experimental indentation based measurements discrimination between physical effects and artifacts - primarily due to variation of indenter contact area and extend of stress field - poses the largest challenge. To calculate the surface sensitivity of the indentation moduli, we performed a computational multiscale approach to study the phenomena on different scales. We utilized ab-initio-DFT and molecular dynamics to simulate the mechanical properties, i. e. the surface elastic constants of Si and SrTiO3 ultra-thin films. These results were used to build up a finite-element layer model where the influence of surface stresses in indentation experiments is studied. Additionally, we propose an analytical model that describes the decrease in the moduli due to surface stresses as a function of the contact radius.

O 97.5 Fri 11:30 MA 005

Efficient conformational sampling of complex adsorbates: Basin Hopping in curvilinear coordinates — Konstantin Krautgasser[1], •Chiara Panosetti[1], Dennis Palagin[2], Karsten Reuter[1], and Reinhard Maurer[3] — [1]Technische Universität München, Germany — [2]University of Oxford, GB — [3]Yale University, USA

Continuous computational and methodological advances provide first-principles access to ever larger and more complex adsorbate molecules. The vastly increasing configurational spaces of such molecules nevertheless pose an enormous challenge. Local geometry optimizations of a few chemically motivated adsorption modes are inadequate to sample these spaces and need to be replaced by rigorous global optimization techniques. In those, a crucial role is played by the choice of coordinates representing geometries and trial moves. When aiming for sampling in chemically motivated subspaces the most popular, but physically blind choice of Cartesians is often inefficient. Rather than e.g. testing for adsorption modes of the intact adsorbate, Cartesian trial moves may quickly lead to dissociated structures. We address this by presenting a Basin Hopping (BH) scheme employing Delocalized Internal Coordinates (DICs) suitable for covalently bound systems. In the application to two rather diverse systems we indeed find that such DIC trial moves significantly reduce the sampling efficiency: Retinoic Acid on Au(111) and $Si_{16}H_{16}$ clusters in gas-phase and on Si(001).

O 97.6 Fri 11:45 MA 005

Theoretical study of structure of solid electrolyte interphase — •Sara Panahian Jand and Payam Kaghazchi — Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Solid electrolyte interphase (SEI) is a heterogeneous layer that is formed on the surface of electrodes (e.g. graphite) in Li-ion batteries during the first charging cycles. The SEI layer plays a key role in the safety, irreversible capacity loss, cycle life, and calendar lifetime of Li-ion batteries. Therefore, fundamental understanding of the structure of SEI layer is a prerequisite for developing advanced electrode materials. In this work, we study the structure and growing mechanism of LiF (a main component of a SEI layer) on graphene using density fiunctional theory (DFT) calculations and electrostatic models. DFT calculations show that, independent of being in contact or not with a graphene surface, crystalline-LiF nanoclusters with (100) facets grow in a three-dimensional mode. This result is in agreement with experimental observations [1]. We also find that the stability of LiF nanoclusters can be predicted by a simple electrostatic model [2]. This model can also be used to study other inorganic components of the SEI layer such as Li_2O and Li_2CO_3 [3].

[1] S. Chattopadhyay et al., Chem. Mater., 24, 3038 (2012)
[2] S. Panahian Jand and P. Kaghazchi, J. Phys.: Condens. Matter, 26, 262001 (2014)
[3] S. Panahian Jand and P. Kaghazchi, in preparation

O 97.7 Fri 12:00 MA 005

Linear and Nonlinear excitations of the Plasmonic Nanogap — Anke Horneber[1], Jan Rogalski[1], Jiyong Wang[1], Anne-Laure Baudrion[2], Pierre-Michel Adam[2], Kai Braun[1], Alfred J. Meixner[1], and •Dai Zhang[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Institut Charles Delaunay, Technical University of Troyes

Plasmonic nanogaps of changing geometries, gaps, and material compositions provide tunable model systems to investigate how plasmonic resonance effect participates in the optical or/and electrical excitation of metallic nanoantennas. As the precise control of nanogap distance of less than 10 nm is still a major challenge, pursuing and investigating narrow gaps even down to the quantum regime attract great research interests. We studied the composition-influences on SHG and 2PPL of homo- and hetero- nanodimers [1-3]. By combining scanning probe microscope with a confocal optical microscope, we investigated the linear/nonlinear PL and electroluminescence from narrow plasmonic nanogaps of down to 1 nm. Furthermore, using a fs-scanning near-field optical microscope, we imaged optical gold nanotriangles with less than 30 nm nonlinear resolution based on the different plasmonic nanogaps formed between the scanning tip and different locations at the nanotriangle [4]. References [1] Horneber A., Baudrion A.-L., Zhang, D. et al., PCCP, 2013, 15, 8031. [2] Reichenbach, P., Zhang D., Eng L. et al., Opt. Exp., 2014, 13,15484. [3] Kern A., Zhang D., Meixner A. J. et al., Chem. Soc. Rev., 2014, 43, 965. [4] Horneber A., Braun K., Zhang, D. et al., PCCP, 2014, in revision.

O 97.8 Fri 12:15 MA 005

A suitable tip for TERS? Find it out with photo-induced force microscopy (PiFM). — •Michael Ludemann[1], Anne-D. Müller[1], Falk Müller[1], Derek Nowak[2], and Sung I. Park[2] — [1]Anfatec Instruments AG, Melanchthonstr. 28, D-08606 Oelsnitz (V) — [2]Molecular Vista Inc., 6840 Via Del Oro, CA-95199 San Jose (USA)

Tip-enhanced Raman spectroscopy (TERS) pushes down the spatial resolution of the measurement below the tip diameter and thus way beyond the diffraction limit of focused light.

Obtaining reproducible TERS results is difficult even with a proper setup. One key factor is a suitable tip.

PiFM offers the opportunity to characterize the tip at any time of the experiment. Here, the intensity of a linear polarized laser beam is modulated at a frequency in the range of the cantilever resonance. Illuminating the tip with the focused light induces a detectable dipole-dipole force even on non-metallic samples (e.g. glass). If the tip provides an appropriate near-field enhancement, a double lobe structure associated with the axial focal field created by a high-NA inverted objective lens is obtained while scanning the tip in the fixed laser focus. This way, PiFM can be utilized as a tool to validate the optical properties of the tip and the laser alignment.

The talk explains the physical background of PiFM and presents experimental results on differently prepared TERS tips.

O 97.9 Fri 12:30 MA 005

Background suppression in near-field optical microscopy by generalized lockin detection — •Susanne Hartmann[1], Falk Müller[1], Yi Huang[2], Abeer Al Mohtar[2], Aurélien Bruyant[2], Michael Ludemann[1], and Anne-D. Müller[1] — [1]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz, V. — [2]Laboratoire de Nanotechnologie et Instrumentation Optique, CNRS (FRE 2671), Universite de Technologie de Troyes, 10010 TROYES cedex, France

A detection scheme is presented that allows to simultaneously measure signal amplitude and phase in near-field optical microscopy (SNOM) with the aid of interferometry. The method is based on a phase modulation of the reference arm inside the interferometer followed by a demodulation of the measured signal with specifically chosen trigonometric functions. The output can be understood as generalized lockin technique (GLIA). The GLIA successfully extracts the signal while suppressing the background. In case of an additional tip oscillation at f_r, a further background subtraction is achieved by a preceding amplitude demodulation of the GLIA's input signal at f_r. The calculations are verified by measurements on gold discs. The method is a crucial step for background suppression with applications not only in near-field optical microscopy.