

O 82: Nanostructures at Surfaces: Graphene and Other Aspects

Time: Wednesday 16:00–18:30

Location: REC/PHY C213

O 82.1 Wed 16:00 REC/PHY C213

Sublimation of non-IPR fullerene dimers — ●JÜRGEN WEPPERT¹, LEA HOHMANN¹, ARTUR BÖTTCHER¹, and MANFRED M. KAPPES^{1,2} — ¹Institute of Physical Chemistry, Karlsruhe Institute of Technology (KIT), Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Non-IPR fullerenes were generated in vacuum by electron impact ionization and fragmentation of IPR fullerenes (C60, C70). The corresponding solids were formed by low energy ion beam deposition of the mass-selected C_n cages onto HOPG. The materials grow via formation of a network of covalently interlinked oligomers. This morphology is responsible for the unique properties of these novel materials such as an (n-dependent) band gap, high thermal stability, hardness and Young's modulus.... Recently we found, that the sublimation of some non-IPR solids proceeds via a second channel: in addition to the dominant emission of monomers we also observe the emission of dimers. These show a significantly higher sublimation enthalpy than found for related monomers. Furthermore, we can relate the monomer geometries to the emission intensity in competition with thermal hardening of the network.

O 82.2 Wed 16:15 REC/PHY C213

Amorphous hydrogenated carbon (a-C:H) depositions on polyoxymethylen (POM) - polymer substrate effects for identical depositions — ●CHRISTIAN B. FISCHER, ALBERTO CATENA, LIZ M. RÖSKEN, and STEFAN WEHNER — Department of Physics, University Koblenz-Landau, 56070 Koblenz, Germany

The polymer polyoxymethylene (POM) has been gradually covered with a-C:H films by radio frequency plasma-enhanced chemical vapor deposition (RF-PECVD) with acetylene plasma after initial oxygen plasma cleaning. Both steps were performed on the same sample plate together with selected polymers like high-density polyethylene (HDPE) and polyethylene terephthalate (PET). The focus of this investigation is to study specific effects during an identical carbon coating on these chemically different polymer substrates. Especially the interlayer forming behavior between these two materials is of primary interest. Surface morphology was conducted by atomic force microscopy (AFM), the chemical composition by diffusive reflectance infrared Fourier transform (DRIFT), near-edge X-ray absorption (NEXAFS) and micro-Raman spectroscopy. Findings indicate the absence of a solid interlayer formation for POM as found for the other two polymers. Furthermore, the developing a-C:H network on POM is remarkably different to the carbon film structure on HDPE and PET. Altogether these results reveal that different plastic substrates strongly affect the resulting structure of the a-C:H coating during identical depositions.

O 82.3 Wed 16:30 REC/PHY C213

Recent advances in Secondary Ion Mass Spectrometry in the Helium Ion Microscope — ●FLORIAN VOLLNHALS, DAVID DOWSETT, JEAN-NICOLAS AUDINOT, and TOM WIRTZ — Advanced Instrumentation for Ion Nano-Analytics (AINA), Luxembourg Institute of Science and Technology (LIST), L-4422 Belvaux, Luxembourg

The Helium Ion Microscope (HIM) has become an ideal tool for imaging with an ultimate resolution down to 0.5 nm using He and nanopatterning of structures with sub 20 nm feature using Ne ions. [1]

As standard analytical techniques like EDX are not compatible with HIM, we have developed a Secondary Ion Mass Spectrometry (SIMS) add-on for Zeiss' Orion Nanofab. [2] SIMS is based on the identification of characteristic secondary ions emitted due to the irradiation of a surface with a primary ion beam. As the probe size in the HIM is substantially smaller (both for He and Ne) than the sputtering interaction volume, the lateral resolution is limited only by fundamental considerations and not by the probe size. The available mass range of up to 500 amu in combination with a mass resolution greater than 400 allows for compositional analysis of nanoscale structures.

We will present our progress in instrumental and method development of HIM-SIMS as well as data obtained on the prototype systems. He and Ne ion beams will be shown to be viable primary species for SIMS, approaching the physical resolution limits of <20 nm.

[1] L. Scipioni et al., J. Vac. Sci. Technol. B 27 (2009), 3250

[2] T. Wirtz et al., in "Helium Ion Microscopy", Springer (2016), p. 297-323

O 82.4 Wed 16:45 REC/PHY C213

Amorphous TiO₂ Inverse Opal Anode for High-rate Sodium Ion Batteries — ●MIN ZHOU, YANG XU, LIYING LIANG, HUAPING ZHAO, BENRONG HAI, and YONG LEI — Ilmenau University of Technology, Ilmenau 98693, Germany

With the increased demands of available energy, potential applications of sodium-ion batteries have motivated significant progress in energy storage field. Compared with Li ions, large radius of Na ions results in different electrochemical behaviors. Hence, synergistic understanding of the differences is greatly significant. Surface availability of ions is critical to rate performance in SIBs. Here, amorphous TiO₂ inverse opal is employed as a proof-of-concept example to illuminate the influences of surface ion availability and the relationship between solvent wettability and rate capability. Enhanced solvent wettability contributes to superior rate capabilities, regardless of the type of electrolyte and the ion concentration in electrolyte. Our concept offers a potential to realize full potential of designing electrode materials for SIBs by adjustable surface kinetics. Similar attentions may be used to mitigate problems caused by ion affinity or other limitations from tremendous Na ions, and enable sodium-ion batteries to be more amenable for large-scale implementations.

O 82.5 Wed 17:00 REC/PHY C213

An extended continuum model for epitaxial growth of graphene: A phase field crystal approach — ●RAINER BACKOFEN¹, SAI TANG², and AXEL VOIGT¹ — ¹Institut für Wissenschaftliches Rechnen, TU Dresden, 01062 Dresden, Germany — ²MPI für Eisenforschung, 40237 Düsseldorf, Germany

Epitaxial growth of graphene on single crystalline metal substrates lead to a large variety of different shaped graphene flakes. E.g. hexagonal, rectangular or butterfly shaped flakes are observed depending on the symmetry of the substrate. This macroscopic morphologies of the crystal have been successfully reproduced by a phase field model following the ideas of step flow modeling introduced by Burton, Cabrera and Frank [1]. In this model, the anisotropy of adatom diffusion and line energy of the growing crystal is adjusted to achieve the different morphologies. We present a phase field crystal model (PFC), that directly introduce the interaction with the substrate on the atomistic length scale and lead to different growth shapes. Thus, the anisotropy of the macroscopic properties are a direct result of the interaction with the substrate. Additionally, defects and elastic deformations are naturally included. This approach combines a multimode extension of PFC, [2], to account for the crystalline structure and a vapor phase PFC model, [3], to control the phase transition at the substrate. With this model we can show how the local interaction to the substrate leads to different shapes of the growing crystal.

[1] Esteban et al., Nano Lett., 2013, 13(11) [2] Mkhonta et al., PRL 111, 035501 [3] Schwalbach et al., PRE 88, 023306

O 82.6 Wed 17:15 REC/PHY C213

Graphene on Ir(110), a twofold-symmetric substrate for van der Waals epitaxy applied to growth of organometallic nanowires — ●FELIX HUTTMANN, STEFAN KRAUS, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Germany

Standard substrates for van der Waals heteroepitaxy, such as graphene on hcp or fcc metal surfaces or H-terminated Si, all possess threefold or sixfold rotational symmetry, and if an adsorbed film does not have such symmetry, this leads to the formation of rotational domains, in conflict with the common goal to achieve an effectively single-crystalline film. We have encountered this problem in the growth of carpets of organometallic nanowires of europium cyclooctatetraene (EuCot) on the graphene/Ir(111) surface, where the lack of a global orientation of the nanowires forbids the study of orientation-dependent properties using spatially averaging techniques. Here, we investigate the growth of graphene on Ir(110), a surface with only twofold rotational symmetry. While clean Ir(110) exhibits faceting, exposure to ethylene at elevated temperatures leads to re-flattening of the surface. Two well-ordered overlayer phases are formed depending on the growth temperature of

either 1250 K or 1380 K. The high-temperature phase is atomically flat over terrace sizes on the order of 100 nm and permits to grow the EuCot nanowires oriented along the [001] direction of the substrate. A single global orientation of almost all nanowires is thus achieved as intended. On the scale of a few hundred nanometers, a structure of ridges and valleys with step edge bundles in between limits the smoothness of the graphene/Ir(110) surface and provides room for improvement.

O 82.7 Wed 17:30 REC/PHY C213

Atomic structure and element distribution of graphene/Ir(111) supported Pt/Rh metal clusters — ●DIRK FRANZ^{1,2}, NILS BLANC^{3,4}, JOHANN CORAUX⁴, HESHMAT NOEI², ROMAN SHAYDUK², and ANDREAS STIERLE^{1,2} — ¹Universität Hamburg, D-20355 Hamburg, Germany — ²DESY NanoLab, D-22607 Hamburg, Germany — ³Institut NEEL, CNRS, F-38042 Grenoble, France — ⁴CEA-UJF, INAC, F-38054 Grenoble, France

Ultrasmall metallic nanoparticles exhibit altered structural, chemical and magnetic properties as compared to their bulk counterparts making them attractive for applications as highly active heterogeneous catalysts or high storage density magnetic media. To pinpoint structure-functionality relationships for systems containing nanoparticles with diameters smaller than 2 nm an atomic scale understanding of their structure is mandatory.

It was previously shown that different 2D metal cluster arrays can be grown using the moiré of graphene/Ir(111) as a template [1]. We have employed several surface sensitive techniques (SXRD, GISAXS, XPS) to investigate the structure of Pt/Rh particles (shape, epitaxy, strain, element distribution) with less than 50 atoms after growth on a graphene/Ir(111) support and in oxidizing/reducing gas environments. SXRD and GISAXS benefits essential from the ordered arrangement of the clusters and is able to reveal the average atomic structure of these small clusters.

[5] A. T. N'Diaye, et al., *New J. Phys.* 11, 103045 (2009).

[6] D. Franz, et al., *Phys. Rev. Lett.* 110, 065503 (2013).

O 82.8 Wed 17:45 REC/PHY C213

Self-assembly of para-hexaphenyl-dicarbonitrile on graphene on Cu(111) — ●NICO SCHMIDT, STEFANO GOTTARDI, JUAN-CARLOS MORENO-LOPEZ, JUN LI, LEONID SOLIANYK, LETICIA MONJAS GOMEZ, ANNA HIRSCH, and MEIKE STÖHR — University of Groningen, Groningen, the Netherlands

Graphene is a 2D material exhibiting various outstanding features. Self-assembled molecules on graphene are often studied with respect to altering the electronic properties, i.e., making graphene more suitable for applications. However, the underlying substrate, on which graphene is grown, has been shown to still have an impact on the formation of the molecular adlayer.

In this study, para-hexaphenyl-dicarbonitrile was deposited onto graphene grown on Cu(111) via chemical vapor deposition. The resulting densely-packed network was found to be stabilized by a combination of dipolar coupling and hydrogen bonding. However, the molecular assembly showed no correlation with the varying orientation of the underlying graphene. This showcases the necessity to carefully assess the influence of the substrate in molecule/graphene interfaces. All experiments were carried out under UHV conditions using low-temperature scanning tunneling microscopy and low-energy electron

diffraction.

O 82.9 Wed 18:00 REC/PHY C213

Electronic and optical properties of ultra-thin graphene nanoribbons — ●BORIS SENKOVSKIY¹, DANNY HABERER², ALEXANDER FEDOROV¹, MARKUS PFEIFFER³, SAYED ALAVI³, NICOLAE ATODIRESEI⁴, VASILE CACIUC⁴, KLAS LINDFORS³, FELIX FISCHER², and ALEXANDER GRÜNEIS¹ — ¹Institute of Physics II, University of Cologne, Germany — ²Department of Chemistry, University of California at Berkeley, Berkeley, USA — ³Institute for Physical Chemistry, University of Cologne, Germany — ⁴Peter Grünberg Institute and Institute for Advanced Simulation, Jülich, Germany

The present work demonstrates that electronic and optical properties of ultra-thin graphene nanoribbons are strikingly different from its 2D or 3D counterparts. A semiconductor-to-metal transition in arm-chair graphene nanoribbons of N=7 carbon atoms width causes drastic changes in the electronic system. By using angle-resolved photoemission spectroscopy of lithium doped nanoribbons, a quasiparticle band gap renormalization from 2.4 eV to 2.1 eV is observed. Reaching high doping levels (0.05 electrons/atom), it is found that the effective mass of the conduction band carriers increases by a factor of four to a value equal to the free electron mass. This giant increase in the effective mass by doping can have palpable impact on the electronic properties of the system. Having carried out the bubble transfer of massively aligned nanoribbons from the gold to the insulating substrate we investigate the optical properties of the material. It is shown that incorporation of sp³ defects induces polarized photoluminescence from intrinsically 'dark' graphene nanoribbons.

O 82.10 Wed 18:15 REC/PHY C213

Formation of Coupled Organic-Inorganic Nanostructures Studied by X-ray Scattering Techniques — ●SANTANU MAITI¹, ALEXANDER ANDRE², MARCUS SCHEELE², and FRANK SCHREIBER¹ — ¹Institute of Applied Physics, University of Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen, Germany — ²Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 18, 72076 Tuebingen, Germany

Electronically coupled hybrid nanostructures of alternating semiconductor nanocrystal (NC) and monolayer of organic semiconductor (OSC) molecules can exhibit interesting charge carrier transport across the superlattice network. Ordered superlattices of coupled organic-inorganic nanostructures (COINs) are a promising material class to realize and exploit the directional transport as well as exciting optical properties^{1,2}. A combined x-ray reflectivity and grazing incidence scattering (GISAXS and GIWAXS) study during COINs formation (ex- and in-situ) of PbS NCs with different OSCs (CuTAPc/TTFDA) has been carried out³⁻⁵. The assembly of nanoparticles and their ordering before and after the ligand exchange process at the air-liquid interface has been monitored. A significant change of about 0.6 and 0.5 nm along the in-plane and out-of-plane direction respectively has been observed after COINs formation. 1. M. P. Boneschanscher et al., *Science* 344, 1377 (2014); 2. M. Scheele et al., *PCCP* 17, 97 (2015); 3. S. Maiti et al., *J. Phys.: Condens. Matter*, 25, 395401 (2013); 4. J. Novak et al., *ACS Appl. Mater. Interfaces* 8, 22526 (2016); 5. A. Andre et al., *Chem. Mater.* 27, 8105 (2015).