

CPP 9: Nanoparticles, Nanocrystals and Composites II

Time: Monday 15:00–16:30

Location: H41

CPP 9.1 Mon 15:00 H41

Tailoring metal nanoparticle layers at the polymer-metal interface — ●STEPHAN V. ROTH¹, MATTHIAS SCHWARTZKOPF¹, OLEKSANDR POLONSKYI², ALEXANDER HINZ², THOMAS STRUNSKUS², FRANZISKA LÖHRER³, VOLKER KÖRSTGENS³, FRANZ FAUPEL², and PETER MÜLLER-BUSCHBAUM³ — ¹DESY, Notkestr. 85, 22607 Hamburg — ²CAU zu Kiel, Kaiserstr.2, 24143 Kiel — ³TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Organic photovoltaic cells, flexible electronics and sensors crucially rely on nanostructuring of thin films at the polymer-metal interface [1]. Here, vacuum deposition of metal layers offers a versatile route for fabricating tailored metal arrays, ranging from isolated nanoparticles to full scale electrical contacts. The interaction of the metal atoms with the underlying polymer template (e.g. wetting) as well as the relevant deposition conditions (e.g. deposition rate and bias-voltage) play a crucial role and influence both the metal layer growth and the development of the near-surface interface in the polymer-metal nanocomposite. We observe in real-time the industrial relevant aluminium layer installation in the different growth modes from nucleation to percolation during sputter deposition on polymer template. Combining in-situ x-ray scattering and ellipsometry, we thus correlate the structural and morphological characteristics of the polymer-metal interface with its optical properties. [1] Roth et al., ACS. Appl. Mater. Interfaces 7, 12470 (2015), & J. Appl. Cryst. 48, 1827 (2015)

CPP 9.2 Mon 15:15 H41

In-situ investigation of aluminum thin film growth on a nanostructured diblock copolymer substrate — ●BJÖRN BEYERSDORFF¹, MATTHIAS SCHWARTZKOPF¹, DENIZA CHEKRYGINA², VALENTIA CANTELLI³, EZZELDIN METWALLI⁴, SENLIN XIA⁴, CARSTEN BAEHTZ^{1,3}, PETER MÜLLER-BUSCHBAUM⁴, and STEPHAN V. ROTH¹ — ¹DESY, Hamburg — ²Universität Hamburg — ³Helmholtz-Zentrum Dresden-Rossendorf — ⁴Technische Universität München

Targeted installation of nanostructured metal films for application devices is of utmost importance in many areas of modern science and technology. Aluminum (Al) nanostructures for instance are very promising for surface-enhanced Raman Scattering (SERS) due to their wide tuneability of the plasmon resonance from the deep UV to the infrared region [1].

When depositing metal on a nanostructured diblock copolymer substrate, a different adatom mobility on the two polymer blocks often leads to selective wetting and thus to nanostructure formation [2,3]. We investigated the sputter deposition of Al on a PS-b-PMMA diblock copolymer thin film by means of grazing incidence small-angle X-ray scattering (GISAXS). The resulting GISAXS pattern yield information on the different growth regimes during nanostructural evolution as well as on the modification of the diblock copolymer substrate due to the Aluminum deposition. [1] Gérard et al, J. Phys. D: Appl. Phys., 48, 184001 (2015), [2] Lopes et al, Nature 414, 735 (2001), [3] Roth et al, ACS Appl. Mater. Interfaces 7 (23), 12470 (2015)

CPP 9.3 Mon 15:30 H41

When do clusters start to behave like a solids: A density-functional theory study of noble gas clusters — ●LYDIA NEMEC², BENJAMIN JOHNSON¹, OLIVER T. HOFMANN³, ALEXANDER M. BRADSHAW⁵, and PATRICK RINKE⁴ — ¹Fritz-Haber-Institut der MPG, Berlin — ²Technische Universität München — ³Technische Universität Graz, Austria — ⁴Aalto University, Helsinki, Finland — ⁵MPG für Plasmaphysik (IPP), Germany

Weakly bonded argon clusters are a popular model system for studying the transition from molecular to bulk behaviour. Angle-resolved photoemission spectra exhibit bulk-like energy dispersion for clusters as small as 200 atoms [1]. To investigate this observation, we performed a density functional theory (DFT) study of Ar and Kr clusters using the all-electron, numeric, atom-centered basis function code FHI-aims. We use semilocal density functionals including van der Waals dispersion terms in the Tkatchenko-Scheffler approach (PBE+vdW). We developed a method to translate cluster states to a *k*-resolved energy dispersion based on a Fourier transformation of the eigenstates. For low-energy structures taken from the structure database [2], we show that already clusters in the 200 atom size range exhibit a bulk-like

atomic structure. We then demonstrate the emergence of a band-like energy dispersion with increasing cluster size. Finally, we discuss the influence of spin-orbit splitting by contrasting Ar with Kr.

[1] Förstel, *et. al.*, J. El. Spec. Rel. Ph. 184, 107-112 (2011) [2] Y. Xiang, *et. al.*, J. Phys. Chem. A, 108, 3586-3592 (2004)

CPP 9.4 Mon 15:45 H41

Nucleation and Growth Kinetics of Multinary Nanocrystals by Quick Extended X-ray Absorption Fine Structure — ●JUSTUS JUST^{1,2}, OLIVER MÜLLER², CLAUDIA COUGHLAN³, KEVIN M. RYAN³, DIRK LÜTZENKIRCHEN-HECHT², RONALD FRAHM², and THOMAS UNOLD¹ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Bergische Universität Wuppertal, Gaußstraße 20, 42109 Wuppertal, Germany — ³Materials and Surface Science Institute and Department of Chemical and Environmental Sciences, University of Limerick, Limerick, Ireland

Early stage nucleation and subsequent growth of multinary nanocrystals (Cu_2ZnSnS_4) are investigated by real time in-situ measurements of the X-ray absorption fine structure at the Cu and Zn K-edges in conjunction with simultaneously measured small angle X-ray scattering and optical transmission. The specially designed hot-injection reaction setup as well as the QEXAFS experimental setup allows to investigate the chemical reaction within timescales of several 10 ms which especially enables the investigation of early reaction stages. We found the monodispersed rod shaped hexagonal nanocrystals to grow within six well distinguishable reaction stages, the kinetics of which are influenced by the choice of ligands and solvents.

CPP 9.5 Mon 16:00 H41

Characterization of active iron sites in Fe-ZSM-5 catalysts using Mössbauer spectroscopy — ●KYDALA GANESHA PADMALEKHA¹, HEMING HUANG¹, INGA ELLMERS², ROXANA PÉREZ VÉLEZ³, ANGELIKA BRÜCKNER³, WOLFGANG GRÜNERT², and VOLKER SCHÜNEMANN¹ — ¹Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — ²Lehrstuhl Technische Chemie, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany — ³Leibniz-Institut für Katalyse e. V., 18059 Rostock, Germany

Fe-ZSM-5 catalysts are important in catalytic reduction of NOx by NH3 in vehicle exhausts. The iron centres in the heterogeneous catalyst can exist in various forms and oxidation states after iron loading and pretreatment and it is non trivial to identify and quantify them. We have investigated isotopically enriched 57Fe-ZSM-5 (Si/Al ~ 14, <= 0.7 wt% Fe), which was prepared via solid-state ion exchange, before and after standard selective catalytic reduction SCR (sSCR) using field dependent Mössbauer spectroscopy. We present deconvolution of the spectra into contributions from the different iron species and their corresponding abundances. We use a five component analysis of the spectra using ferric iron oxide, ultrasmall ferric iron agglomerates a part of which are diamagnetic, paramagnetic ferrous high spin ions and two kinds of paramagnetic ferric high spin ions which were detected using EPR spectroscopy.

CPP 9.6 Mon 16:15 H41

BaTiO3 Modifications for Photochemical Hydrogen Evolution — ●YAN XIONG and FRANK MARLOW — Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

The perovskite-type material BaTiO3 is a wide-bandgap semiconductor and a prospective material for the photochemical hydrogen evolution via water splitting. In our work, we studied reduction-treatments of BaTiO3 and the effect of Pt as a co-catalyst on BaTiO3 for the hydrogen evolution reaction. We found that the catalytic activity of reduced-BaTiO3 is enhanced by a factor of 1.5 compared to the original material. The rates of hydrogen generation of reduced and bare BaTiO3 are 159 and 100 $\mu\text{mol/h}$, respectively. The effect of Pt as a co-catalyst on BaTiO3 is non-linear. The photocatalytic activity increases up to 527 $\mu\text{mol/h}$ with the increasing Pt amount up to 1 wt.% and decreases above this amount. In our study reduced BaTiO3 with 1 wt.% Pt has shown the best performance.