CPP 8: Poster: New Instruments and Methods

Time: Monday 17:30–19:30 Location: Poster C

CPP 8.1 Mon 17:30 Poster C

P62: A new small angle X-ray scattering instrument for the PETRA III Extension — •Jan Perlich, Jan Rubeck, Rainer Gehrke, and Sergio Funari — Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg (Germany)

Presently PETRA III is the most brilliant storage-ring-based X-ray radiation source in the world and thereby offers outstanding conditions for experiments with X-rays featuring small beam cross sections, high degree of collimation, and a wide range of photon energies. In the next years, the experimental facilities at PETRA III will be extended to provide additional instruments for various applications. This PETRA III Extension project will accommodate the new small angle X-ray scattering (SAXS) beamline P62 which is intended to comprise the large variety of X-ray scattering methods ranging from wide angle X-ray scattering (WAXS) to high-resolution ultra-small angle X-ray scattering (USAXS) in transmission and reflection geometry. Furthermore, the new instrument shall allow exploitation of anomalous X-ray scattering (ASAXS) with all setups and provide the option for simultaneous measurement in different angular scattering regimes. Due to the high photon flux available, time-resolved experiments down to milliseconds temporal resolution will be possible. We will present the characteristics and design parameters of the instrument and give a comprehensive overview of the experimental possibilities opened with this new instrument.

CPP 8.2 Mon 17:30 Poster C

Fluorescence Lifetime Imaging Microscopy in the Frequency Domain — •Stephanie Zahner[1], Lothar Kador[1], Inga Elvers[1], Jürgen Köhler[1], Kerim R. Allahverdi[2], and Eldar Yu. Salaev[3] — [1]University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), Bayreuth, Germany — [2]Marmara Research Centre of TÜBITAK, Materials Institute, Gebze/Kocaeli, Turkey — [3]Azerbaijan National Academy of Sciences, Institute of Physics, Baku, Azerbaijan

A custom-built, low-cost Fluorescence Lifetime Imaging Microscope (FLIM) working in the frequency domain has been optimized and tested with three different materials. In addition to two-dimensional FLIM images, the results are shown in polar plot representation. Polymer matrices (PMMA and PVA) doped with Rhodamine 6G were used for characterizing the setup and the evaluation method. Films of the organic polymeric semiconductor P3HT show a distribution of short lifetimes below one nanosecond in combination with a longer lifetime component. The data points of the layered chalcogenide semiconductor Gallium-Selenid (GaSe) are spread over a wide range in the polar plot, some of them lying distinctly outside the semicircle. This effect is ascribed to the superlinear variation of the material's photoluminescence with the excitation light and has not been described in literature before.

CPP 8.3 Mon 17:30 Poster C

Characterization of heavy ion induced defects in ionic crystals by magnetic resonance techniques — •Michael Ditter, Kai-Christian Meyer, Sebastian Orth, and Franz Fujara — Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt

We explore the potential and limitations of nuclear magnetic resonance (NMR) as a tool for the examination of heavy ion induced radiation damage in materials. We choose various fluoride crystals as guinea pig systems, here focusing at lithium fluoride (LiF). LiF offers two suitable probe nuclei for NMR, further on paramagnetic defects, such as F-centers, and metallic colloids can be observed directly by electron spin resonance (ESR). Extensive research has been carried out in the past but has also lead to new unanswered questions. NMR relaxometry with one dimensional spatial resolution is used to study defect generation and annealing behavior as well as impurity cluster formation along and beyond the ion path. Data from conventional and spatially resolved NMR field-cycling experiments, the latter with a purposely built spectrometer [1], can be utilized to determine defect distribution. NMR spectroscopy is used to observe fluorine gas bubbles formed during irradiation. Additionally CW ESR allows us to measure the density of paramagnetic defects as well as the formation of higher F-center aggregates, lithium and impurity colloids during annealing experiments. The latest results will be presented.

[1] M. Ditter, H. Stork, B. Schuster, F. Fujara: Journal of Magnetic Resonance 209 (2011) 47-52

CPP 8.4 Mon 17:30 Poster C

Scanning force microscopy and polarized confocal- RAMAN microscopy for in-situ characterization of uniaxially stretched ethylene based thermoplastic elastomers — •Jörg Mühlböck, Krisztina Vincze-Minya, and Sabine Hild — Institute of Polymer Science, Johannes Kepler University, Linz, Austria

Polyethylene based elastomers are low crystalline materials which show interesting elastic mechanical behavior due to physical crosslinking. Nevertheless, the morphology of these polymers is still sparsely resolved. For a better understanding of the unique mechanical properties, microscopic changes in morphology and strain-induced variation in chain orientation of two polyethylenes with statistically distributed octene or butene side chains were monitored during uniaxial stretching using scanning force microscopy (SFM) and polarized Raman microscopy. For these purpose a stretching device has been developed and integrated in an existing SFM to visualize differences between an unstretched and stretched sample. Additionally, the set-up will be used to determine crystallinity and orientation of the samples before and after deformation via polarized Raman microscopy and polymer chain orientations were calculated for quantitative analysis. The correlation between the orientation, the arrangements of the amorphous and crystalline phases and the mechanical properties of the material at different elongation ratios allowed an interpretation of the macroscopic behavior on the microscopic scale.

CPP 8.5 Mon 17:30 Poster C

Border Search - Robust potential energy surface mapping technique — •Prokop Hapala and Pavel Jelinek — Institute of Physics , Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague, 16253, Czech Republic

Mapping of Potential Energy Surface (PES), searching for local and global minima of atomistic systems or paths with minimal energy barrier between these local minima is a long term goal of computational chemistry and material science. We propose novel robust method inspired by Metadynamics [1] providing advantages in several aspects: (a) No force evaluation is needed. (b) Positions in configuration space are sampled systematically and homogeneously. (c) Method setup has less parameters and is easier to control. (d) Lowest energy barrier is always found. (e) Number of PES evaluations required to reliable exploration of lowest energy path to neighboring local minimum is reduced by prohibiting re-examination of the same area.

[1] B. Ensing, et. al. Metadynamics as a tool for exploring free energy landscapes of chemical reactions. Acc. Chem. Res., 39, 73-81 (2006).

CPP 8.6 Mon 17:30 Poster C

Determination of the Modulation Transfer Function in a Holographic 2D-Data Storage System — •Christoph Meichner[1], Lothar Kador[1], Christian Probst[2], and Hans-Werner Schmidt[2] — [1]University of Bayreuth, Institute of Physics and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and Bayreuther Institut für Makromolekülforschung (BIMF), 95440 Bayreuth, Germany

A holographic storage set-up was improved and characterized which is able to inscribe entire data pages into azobenzene-based media by means of a spatial light modulator (SLM). For the quantitative characterization of the imaging quality a fast and reliable method is required, which does not need every digital bit to be read out. To this end a simple measurement was performed which is based on the determination of the contrast of different periodical structures displayed on the SLM. The change in contrast of sinusoidal intensity patterns transferred through the optical system is analyzed with the hologram read-out camera in two directions perpendicular to the optical axis. The contrast as a function of the spatial frequency displayed on the SLM provides the data to calculate the modulation transfer function of the system. The experiments demonstrate the optical limitations of the set-up and the degree by which they are affected by the storage medium. In this way they yield information about the amount of

storable data which is one of the key quantities in holographic data storage.

CPP 8.7 Mon 17:30 Poster C

Applications of Infrared Transition Moment Orientational Analysis (IR-TMOA) — •Wilhelm Kossack[1], Wycliffe Kiprop Kipnusu[1], Periklis Papadopoulos[2], Malgorzata Jasiurkowska[3], and Friedrich Kremer[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Abteilung Molekülphysik, Linnestr. 5, 04103 Leipzig, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55021 Mainz, Germany — [3]The Henryk Niewodniczanski Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland

IR-TMOA is a recently developed experimental technique that enables one to determine the full *three dimensional* molecular order parameter tensor with respect to a sample coordinate system (reflecting degree of order and mean orientation directions). Relying on the dependence of the IR spectra on polarization *and* an intentional inclination of the sample with respect to the optical axis, specific information for the various molecular moieties in any IR translucent material can be obtained. The approach is of fundamental interest in polymer science and industry[1], for liquid crystal applications[2,3], organic electrets and it can provide insight into interactions in confined geometries[2,4]. We will present examples from each of these fields emphasizing the multiple opportunities of this technique.

[1] Kossack, W. et al. *Polymer* 52, 6061 (2011). [2] Jasiurkowska, M., W. Kossack et al. *Soft Matter* 8, 5194 (2012). [3] Kossack, W. et al. *Macromolecules* 43, 7532 (2010). [4] Kipnusu, W. K., W. Kossack et al. *Zeitschrift für Physikalische Chemie* 226, 797 (2012).

CPP 8.8 Mon 17:30 Poster C

Dynamic SEM image analysis of vibrating cantilevers (I) — •Maria-Astrid Schröter[1], Matthias Holschneider[2], Christiane Weimann[1], Martin Ritter[3], and Heinz Sturm[1] — [1]BAM 6.9, Federal Inst. Materials Research, Berlin — [2]Inst. Mathematics, Univ. Potsdam — [3]Electron Microscopy TU Hamburg-Harburg

SFM cantilevers excited to vibration are used to perform intermittent- or non-contact modes or serve in force modulation techniques and derivatives thereof. Even sub-atomic resolution was demonstrated already. Advanced techniques include multi-frequency excitation for the use of higher modes to improve sensitivity or to examine tip-sample interactions related to materials properties. In all methods, non-linear effects can appear giving rise to harmonics of excitation frequency. The technique presented here named Dynamic Scanning Electron Microscopy (DySEM) enables us to image shapes of vibrating structures in different modes in terms of amplitude and phase shift measured by a lock-in amplifier (1,2). Our contribution concentrates on experimental issues and in this is part (I) the method is introduced and pictures of different modes and harmonics are presented. For the first time, the resulting motion induced by multiple frequency excitation (f_1, f_2) is imaged at the sum (f_1+f_2) and difference (f_1-f_2) frequency. The mathematical analysis and a new developed model is presented in a second poster (II).

(1) Schröter, Holschneider, Sturm; Nanotechn. 23, 435501 (2012).
(2) Sturm, Schröter, Weimann; Microelectr. Eng. 98, 492 (2012).

CPP 8.9 Mon 17:30 Poster C

Dynamic SEM image analysis of vibrating cantilevers (II) — •Maria-Astrid Schröter[1], Matthias Holschneider[2], Christiane Weimann[1], Martin Ritter[3], and Heinz Sturm[1] — [1]BAM 6.9, Federal Inst. Materials Research, Berlin — [2]Inst. Mathematics, Univ. Potsdam — [3]Electron Microscopy TU Hamburg-Harburg

Dynamic Scanning Electron Microscopy (DySEM) is used to examine vibration modes and their harmonics at flexural and torsional resonance (1). In this part (II), the mathematical analysis of the imaging mechanism of DySEM is explained in detail. Recently, we presented a new model (2) describing the dynamic interaction of an electron beam with a periodically vibrating cantilever to explain and reproduce the topological features of amplitude images. Here we present an extended model taking into account the full periodic space-time dynamics i.e., amplitudes (moduli) and phase shifts as well as real and imaginary parts. A general methodology is demonstrated to distinguish non-linear features caused by the imaging process from those caused by cantilever motion. To describe complex dynamic contact behaviour, signal amplification is needed to enable measurements with a resolution below 10 nanometres. Strategies to improve image quality and sensitivity are discussed.

(1) Sturm, Schröter, Weimann; Microelectr. Eng. 98, 492 (2012).
(2) Schröter, Holschneider, Sturm; Nanotechn. 23, 435501 (2012).

CPP 8.10 Mon 17:30 Poster C

V16/VSANS - a new tool for soft matter research at the HZB — •Miriam Siebenbürger, Daniel Clemens, and Karsten Vogtt — Helmholtz Zentrum Berlin, Berlin, Deutschland

We would like to present the possibilities of the Time of Flight Small Angle Neutron Scattering beamline of the HZB, regarding the q-range, resolution and sample environment. Due to the use of different choppers, the q-range and resolution can be variied. First measurements of Soft Matter samples (colloids, polymers and proteins) will illustrate the performance of the VSANS. Furthermore, the availible sample environments will be presented: a temperature controlled mulit-sample holder, a sample cell with a very accurate temperature stability and a Rheo-SANS environment.

CPP 8.11 Mon 17:30 Poster C

The multipurpose hard x-ray beamline BL9 at DELTA — •Thomas Büning, Michael Paulus, Christian Sternemann, and Metin Tolan — Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund

The hard x-ray beamline BL9 ls located at the synchrotron radiation facility DELTA (Technische Universität Dortmund). Here, x-ray scattering studies can be performed using radiation in the energy range 4 - 30 keV provided by a superconducting asymmetric wiggler. The x-rays are monochromatized by a sagittally focusing Si (311) double crystal monochromator and the experimental endstation is equipped with a Huber six-circle diffractometer. At the beamline several detection schemes are available using point detectors, a MAR345 image plate scanner, or Pilatus 100 K area detector allowing for various x-ray scattering experiments such as (grazing incidence) x-ray diffraction, x-ray reflectivity, and small angle x-ray scattering. The beamline layout will be presented and different experiments will be discussed to emphasize the capabilities of the instrument.

CPP 8.12 Mon 17:30 Poster C

Microfluidics and microGISAXS - nanoscopic in situ characterization at the solid-liquid interface — •Volker Körstgens[1], Martine Philipp[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

We present an experimental microfluidic technique which allows for versatile structural investigations at the solid-liquid interface with high time resolution. In our approach reflection geometry using GISAXS (grazing incidence small angle x-ray scattering) is combined with a special designed microfluidic cell where the nanostructures at the solid-liquid interface are investigated. With the microfocussing of the highly brillant x-ray beam of a third generation synchrotron source the kinetics of different processes in the nanoscopic regime are accessible. Applications include the investigation of attachment processes as in the layer formation of nanoparticles, detachment processes of unwanted detrimental films, as well as mixing and swelling experiments. Details on how to adjust the experimental settings (e.g. the beamsize) to the respective addressed questions will be given.

This work has been financially supported by the BMBF (grant number 05K10WOA).

CPP 8.13 Mon 17:30 Poster C

First-principles calculation of non-adiabatic coupling vector — Pavel Jelinek[1], Enrique Abad[2], •Vladimír Zobač[1], Prokop Hapala[1], James Lewis[3], and José Ortega[2] — [1]Institute of Physics of the Czech Academy of Science, Prague, Czech Republic — [2]Universidad Autónoma de Madrid, Madrid, Spain — [3]West Virginia University, Morgantown, United States

Many of the chemical reactions and physical phenomena going beyond the Born-Oppeinheimer approximation (B-O) are not possible to describe by conventionally first principles Molecular dynamics (MD) within (B-O) approximation. These phenomena need to describe not only ground state potential energy surface (PES), but also the excited one. The central quantity of such simulations is nonadiabatics-coupling

vector (NAC), which allow us to describe correctly MD of the excited states.

The direct calculation of NAC based on local-orbital density functional theory has been recently implemented into Firaball code [1] together with time dependent Kohn-Sham dynamics within fewest switches surface hopping approximation [2,3] . Here we describe computationally efficient algorithm. We will present several cases of studies to demonstrate applications of this technique.

[1] J.P. Lewis et al, Phys. Stat. Sol. B, 248, 1989 (2011) [2] J. C. Tully, J. Chem. Phys. 93, 1061 (1990); C.F. Craig et al, Phys. Rev. Lett. 95, 163001 (2005). [3] N. L. Doltsinis. in John von Neumann Institute for Computing (NIC) Series (ed. J. Grotendorst, D. M., and A. Muramatsu) 377-397 (2002).

CPP 8.14 Mon 17:30 Poster C

a cold chopper spectrometer for ESS — •Luca Silvi[1,2], Wiebke Lohstroh[1,2], Giovanna Simeoni[1,2], Jürgen Neuhaus[1,2], and Winfried Petry[1,2] — [1]Technische Universität München - Physik Department E13 — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II)

The European Spallation Source (ESS) will provide a high neutron flux, comparable to the best existing steady state reactors. The proposed cold direct time-of-flight spectrometer is a versatile instrument to address important scientific cases, ranging from soft matter and biological samples to magnetic and functional materials. These materials show motions on different length and time scales, requiring an instrument with flexible to high energy resolution and a broad accessible q-range. With the maximum pulse length of $1000\mu s$ (FWHM) usable for a clean resolution function, an energy resolution of 100μeV at $5\AA$ is expected, with the possibility to reach $5-10\mu$eV at $9\AA$. The natural bandwidth usable for any experiment in Rate Repetition Multiplication (RRM) mode is $2.6\AA$, covering a reasonable part of $S(\mathbf{q},\omega)$ in one measurement. The chopper and guide system of proposed instrument will be optimized for cold neutrons and will foresee the use of dedicated sample environments (polarization analysis, magnetic fields).

CPP 8.15 Mon 17:30 Poster C

Bispectral powder diffraction at the long pulse source ESS — •Nicolò Violini[1], Werner Schweika[1,2], Andreas Houben[3], Klaus Lieutenant[4], and Paul F. Henry[2] — [1]JCNS, Forschungszentrum Jülich GmbH, D-52425 Jülich Germany — [2]European Spallation Source ESS AB, Lund, Sweden — [3]RWTH Aachen University, Germany — [4]Helmholtz-Centre Berlin, Germany

Within the ESS Design Update Program, funded by the German Federal Ministry of Education and Research, we investigate a versatile instrument concept for powder diffraction at the ESS. Typical applications will be the determination of structures involving light or neighboring elements, complex magnetic structures, and the ability to *in-situ* follow phase transitions in reactive or functional materials, under conditions close to operation. To match the various needs, we investigate a bispectral time-of-flight diffractometer that efficiently makes use of thermal and cold neutrons (0.8-4.6Å). Moreover a wide wavelength spectrum is of interest to exploit the backscattering option with high resolution. The conceptual design utilizes a 10x10mm^2 eye-of-the-needle[1] at 6m from the source, defining an image of 5 to 10 mm diameter with an initial divergence of +/-0.6°. It reduces background by more than two orders of magnitude, as early as possible, thus it helps to design more cost-efficient shielding. It allows to fit in counter rotating disc choppers that are able to provide flexible resolution from 10 μs to 1 ms. The desired phase space is transported by elliptic guides to the sample position of similar size, with only small losses. [1] A. Houben et al., NIMA, 2012, 680, 124.

CPP 8.16 Mon 17:30 Poster C

Perspectives for spectroscopy at the future European Spallation Source — •Nicolò Violini, Jörg Voigt, Thomas Brückel, Earl Babcock, and Zahir Salhi — Jülich Centre for Neutron Science, JCNS, Forschungszentrum Jülich GmbH, ESS Design Update Program - Germany, D-52425 Jülich Germany

Within the ESS Design Update Program funded by the German Federal ministry of Education and Research, we investigate the performance of a multispectral time-of-flight spectrometer at the long pulse source of the ESS, which promises the applicability to a wide manifold of scientific activities of research: strongly correlated electron materials, disordered systems, functional materials, magnetism, soft-matter and biophysics. The concept makes use of a pin-hole 2.5x4.5cm^2 at 6m from the moderator that helps to reduce the background. A powerful double elliptic guide system is able to transport neutron brilliance to a small sample size 1x3cm^2, with a brilliance transfer approaching 1. The chopper system contains fast choppers in the focal points of the ellipses providing unprecedented resolution or intensity depending on the request of the experiment. In combination with the band-width choppers and pulse suppression choppers, the system is perfectly adapted to the requirements of the novel repetition rate multiplication method. The use of polarization analysis for this instrument class is under investigation and its implications will be discussed during the talk.