Workshop on Science of "From Matter to Materials and Life"

14-16. 12. 2016
DESY, Hamburg

Abstracts

Please note:
This collection is based on the abstracts submitted in the registration website (Status Friday, 12 December 2016) and sorted alphabetically by title.
In addition only the primary author is presented.

2-Mercaptopyridine on Excited State Potential Energy Surfaces

Content:

Thione-thiol tautomerism and correlated proton transfer reactions initiate configuration changes of biomolecules e.g. DNA which are vital to life [1,2]. 2-Mercaptopyridine (2-MP) is a model compound which contains building blocks similar to the ones of those biomolecules and exhibits a rich speciation dependent on its chemical environment [3,4]. In this talk the fingerprint of 2-MP speciation on X-ray absorption and emission spectra and 2-MP's ultrafast dynamics on X-ray and optically excited potential energy surfaces will be addressed.

Utilizing nitrogen (N) 1s Near Edge X-ray Absorption Fine Structure (NEXAFS) spectroscopy and Resonant Inelastic X-ray Scattering (RIXS) in liquid jet experiments we gain access to the unoccupied and occupied local valence electronic structure (LVES) at the N site of 2-MP in aqueous solution. We detect the protonation state of the 2-MP nitrogen site and hence the tautomeric equilibrium dependent on the basicity of the solution from shifts in NEXAFS spectra. The impact of N site deprotonation on the occupied LVES is disentangled from RIXS spectra. Especially changes of the overlap between the N 2p lone pair orbital forming the chemical bond to the hydrogen atom in the thione species of 2-MP and the N 1s core hole are detected.
The signatures of ultrafast dynamics upon optical and X-ray excitation of 2-MP are studied exploiting the adjustable scattering duration in the RIXS process and in X-ray/optical pump-probe experiments. The correlated changes of the chemical structure are identified from theoretical calculations of the excited state potential energy surfaces.

[1]
Watson, Crick; Nature 1953, 171 (4356), 737–738.
[2]
Florián, J.; Leszczyński; J. Am. Chem. Soc. 1996, 118 (12), 3010–3017.
[3]
Beak, P.; Acc. Chem. Res. 1977, 10 (5), 186–192.
[4]
Beak, P.; Covington, J. B.; Smith, S. G.; White, J. M.; Zeigler, J. M.; J. Org. Chem. 1980, 45 (8), 1354–1362.

Primary authors:
ECKERT, Sebastian (Institute Methods and Instrumentation in Synchrotron Radiation Research, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH)

Co-authors :
PIETZSCH, Annette (HZB) NORELL, Jasper () ODELIUS, Michael () FöHLISCH, Alexander ()

3D scaffolds for cell culturing by means of phase contrast X-ray computed tomography

Content:

The proliferation mechanisms of cells, especially cancer cells and their responses to drugs, compounds or signaling molecules have been studied by 2D cell culturing for many decades. Limitations of this method have been increasingly recognized over the years [1], the main disadvantage being the inability of the rigid plastic dishes or plastic flasks in which the cells are cultured to reflect the realistic 3D structuring of the cell microenvironment and thus to provide an optimal surrounding for the culturing of established and primary cell lines [2].
On one side, scaffolds represent a valid alternative to 2D culturing systems for studying the normal and pathological behavior of cancer cells (e.g. prostate cancer cells, PCa) thanks to their 3D pore architecture that reflects more closely the physiological environment in which PCa cells develop [3, 4, 5]. This interconnected system of pores provides mechanical stability and mimics simultaneously the 3D cellular environment where the cells, which are to be investigated, can proliferate and differentiate [5, 6].
On the other side, the scaffolds (e.g. PCL polymers) are ideal candidates for regeneration applications, due to controllable degradation rate. Substitution and regeneration of diseased or injured bone tissues by combination of different components, such as biomaterials, hydroxyapatite and cells is now seen as a realistic perspective by developing artificial 3D scaffolds, which help to support the formation of a new tissue by inducing cell adhesion and proliferation [7]. The type of differentiated tissue depends on an appropriate environment, which is surrounding cells. To better adapt the biomaterials properties to the native system of the organism, we developed the scaffolds, which consist of polymer PCL and advanced hydroxyapatite – SiHA components with two different structures (randomly-oriented and well aligned) to mimic the native bone tissues.
The cell proliferation inside scaffolds is typically investigated by using scanning electron microscopy (SEM). This technique provides information only on 2D level without accessing the internal structure of the sample, unless the scaffold is sectioned and thus destroyed. In this perspective, phase contrast x-ray tomography is a unique method of accessing structure of the biomaterials and proliferation of cells. In this work the 3D morphology of the scaffolds was investigated by means of synchrotron X-ray computed micro tomography (SXCμT) fitting the according requirements of high spatial resolution, 3D imaging capability and low dose requirements very well.
References
[1] R. Edmondson, J. Jenkins Broglie, A. F. Adcock, and L. Yang, Assay and Drug Dev. Technologies 12(4) (2014) 207-218.
[2] F. Pampaloni, E. G. Reynaud and E. H. K. Stelzer, Molecular Cell Biology 8 (2007) 839-845.
[3] M. Ravi, V. Paramesh, S.R. Kaviya, E. Anuradha and F.D.P. Solomon, J. Cell. Physiol. 230 (2014) 16-26.
[4] V. I. Lozinsky, I. Y. Galaev, Trends in Biotechnology 21(10) (2003) 445-451.
[5] A. Tripathi, A. Kumar, Macrom. Biosci. 11 (2011) 22-35.
[6] S. Rhee, Experimental and Molecular Medicine 41 (2009) 858-865.
[7] V. I. Lozinsky, I. Y. Galaev, Trends in Biotechnology 21(10) (2003) 445-451.

Primary authors:
Dr. CECILIA, Angelica (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Dr. ALTAPOVA, Venera (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.)

Co-authors :
Mrs. BAECKER, Anne (Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1 Bldg 329, Eggenstein-Leopoldshafen (Karlsruhe), D-76344, Germany.) Dr. HAMANN, Elias (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology,

Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Dr. VAN DE KAMP, Thomas (Laboratory for Applications of Synchrotron Radiation (LAS), Karlsruhe Institute of Technology, 6980, D-76128 Karlsruhe, Germany.) GRUHL, Friederike (Institute of Microstructure Technology (IMT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1 Bldg 329, Eggenstein-Leopoldshafen (Karlsruhe), D-76344, Germany.) Dr. HOFMANN, Ralf (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Dr. MOOSMANN, Julian (Institute of Materials Research, Helmholtz-Zentrum Geesthacht (HZG), Max-Planck-Str. 1, D-21502 Geesthacht, Germany.) Mr. HAHN, Steffen (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Dr. BAUER, Sondes (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Mr. FARAGO, Tomas (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) HELFEN, Lukas (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Prof. BAUMBACH, Tilo (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen.) Mrs. SVETLANA, Gorodzha (Tomsk Polytechnic University (Tomsk)) SURMENEV, Roman (Tomsk Polytechnic University (Tomsk)) Dr. RACK, Alexander (European Synchrotron Radiation Facility (ESRF), 6 rue Jules Horowitz, 38000 Grenoble, France.)

A cryogenic helium buffer gas source for producing cold beams of large biomolecules

Content:

We have designed a cryogenic helium buffer source for producing high flux beams of cold biomolecules [1-3]. These cold beams will be used for many experiments including spatial separations structural isomers of many biomolecules by electrostatic deflection in an inhomogeneous electric field [4]. The structurally pure biomolecules then will be aligned and oriented in the laboratory for determinations of their three dimensional structures by x-ray or electron diffractive imaging [5, 6].
With our new apparatus we have produced cryogenic helium buffer gas cooled beams of NH3 molecules. These NH3 beams have been detected via strong field ionization and time of flight mass spectrometry. We are currently moving towards measuring the rotational temperature of buffer gas cooled NH3 molecules by resonance enhanced multiphoton ionization [7], and cryogenic cooling of large molecules.
The testing and calibration of our cryogenic beam source with NH3 molecules and our progress towards producing cryogenic helium buffer gas cooled beams of large biomolecules will be presented.
References
1. N. R. Hutzler, H.-I Lu, and J. M. Doyle, Chem. Rev. 112, 4803 (2012) 2. David Patterson and John M. Doyle, Phys. Chem. Chem. Phys. 17, 5372 (2015)
3. J. Piskorski, D. Patterson, S. Eibenberger, and J. M. Doyle, ChemPhysChem 15, 3800 (2014)
4. F. Filsinger, J. Küpper, G. Meijer, J. L. Hansen et al., Angew. Chem. In. Ed. Lett. 48, 6900 (2009)
5. J. Küpper, S. Stern, L. Holmegaard et al., Phys. Rev. Lett. 112, 083002 (2014)
6. A. Barty, J. Küpper, H. N. Chapman, Annu. Rev. Phys. Chem. 64, 415 (2013)
7. M.N.R. Ashfold, S.R. Langford, R.A. Morgan et al., Eur. Phys. J. D 4, 189 (1998)

Primary authors:
VIJAY, Singh (DESY)

A new computational tool for describing the behavior of molecules in high-intensity x-ray fields

Content:

Unprecedentedly intense x-ray pulses, provided by x-ray free-electron laser (XFEL) facilities, can create unusual, highly excited states of matter, which have not been conceivable with conventional light sources. I will discuss theoretical and numerical challenges to describe extreme states of matter created by XFEL, and introduce a new computational tool to explore ultrafast explosion dynamics of molecules in high-intensity x-ray fields. It will provide a key insight to understand fundamental XFEL-matter interactions and a basis to design new frontiers of XFEL science.

Primary authors:
Dr. SON, Sang-kil (CFEL, DESY)

Achievements on ex-situ nano-metrology at the BESSY-II-Optics Lab of the Helmholtz Zentrum Berlin

Content:

TTo fully exploit the ultimate source properties of the next generation light sources, such as Free-Electron Lasers (FEL) and Diffraction Limited Storage Rings (DLSR), the requirements on the quality of X-ray gratings and reflective optics, especially beam-shape-transforming (e.g., nano-focusing) mirrors, have significantly increased. In this poster we present recent achievements on ex-situ metrology that allows us to characterize the surface slope variation of super polished optical components like X-ray mirrors with an accuracy better than 50 nrad (root-mean-square), which corresponds to sub-nm accuracy in the height domain. We also discuss a new method based on linear chirped profiles suitable for modulation transfer function (resolution) calibration of slope measuring profilers like the LTP and NOM systems.

Primary authors:
SIEWERT, Frank (Helmholtz Zentrum Berlin)

Co-authors :
BUCHHEIM, Jana (Helmholtz Zentrum Berlin) GWALT, Grzegorz (Helmholtz Zentrum Berlin) ZESCHKE, Thomas (Helmholtz Zentrum Berlin) FALKENBERG, Gerald (DESY) VIEFHAUS, Jens (DESY) ARNOLD, Thomas (IOM) YASHCHUK, Valeriy, V. (LBNL)

Angular correlations between atomic lattice and superlattice of PbS nanocrystals assembled with directional linking

Content:

Coupled organic-inorganic nanostructures (COIN) provide a new approach to applications of semiconductor nanocrystals (NC) for power conversion. A typical COIN consists of periodically alternating NCs and organic semiconductor molecules, promoting carrier transport across the lattice.
By angular x-ray cross correlation analysis (XCCA) we studied the angular correlations between the atomic lattice and superlattice of PbS nanocrystals assembled with directional linking.

Primary authors:
Mr. ZALUZHNYY, Ivan (Deutsches Elektronen-Synchrotron DESY)

Co-authors :
Dr. KURTA, Ruslan (European XFEL GmbH) Dr. ANDRE, Alexander (Eberhard Karls Universität Tübingen) Mr. GOROBTSOV, Oleg (Deutsches Elektronen-Synchrotron DESY) Mr. ROSE, Max (Deutsches Elektronen-Synchrotron DESY) Dr. ZOZULYA, Alexey (Deutsches Elektronen-Synchrotron DESY) Dr. SPRUNG, Michael (Deutsches Elektronen-Synchrotron DESY) Prof. SCHREIBER, Frank (Eberhard Karls Universität Tübingen) Prof. VARTANYANTS, Ivan (Deutsches Elektronen-Synchrotron DESY) Prof. SCHEELE, Marcus (Eberhard Karls Universität Tübingen)

Application of Ion Beams to Fabricate and Tune Properties of Dilute Ferromagnetic Semiconductors

Content:

Combining semiconducting and ferromagnetic properties, dilute ferromagnetic semiconductors (DFS) have been under intensive investigation for more than two decades. Mn doped III-V compound semiconductors have been regarded as the prototype of the type. In this contribution, we will show how the implantation technique, a standard method for doping Si in microelectronic industry, can be utilized in fabricating and deeper understanding of DFS. First, ion implantation followed by pulsed laser melting (II-PLM) provides an alternative to the widely used low-temperature molecular beam epitaxy (LTMBE) approach in the preparation of diverse DFS. The prepared DFS materials exhibit pronounced magnetic anisotropy, large X-ray magnetic circular dichroism as well as anomalous Hall effect and magnetoresistance [1-10]. Going beyond LT-MBE, II-PLM is successful to bring two new members, GaMnP and InMnP, into the family of III-Mn-V. Both GaMnP and InMnP films show clear signatures of ferromagnetic coupling and an insulating behavior. Second, helium ions can be used to precisely compensate the holes while keeping the Mn concentration constant [11, 12]. We monitor the change of Curie temperature (TC) and conductivity. For a broad range of samples including (Ga,Mn)As and (Ga,Mn)(As,P) with various Mn and P concentrations, we observe a smooth decrease of TC over a wide temperature range with carrier compensation while the conduction is changed from metallic to insulating. In the low compensation regime, we can tune the uniaxial magnetic easy axis of (Ga,Mn)(As,P) from out-of-plane to in-plane with an isotropic-like intermediate state. These materials synthesized or tailored by ion beams provide an alternative avenue to understand how carrier-mediated ferromagnetism is influenced by localization.

[1] M. Scarpula, et al., Phys. Rev. Lett. 95, 207204 (2005).
[2] D. Bürger, S. Zhou, et al., Phys. Rev. B 81, 115202 (2010).
[3] S. Zhou, et al., Appl. Phys. Express 5, 093007 (2012).
[4] M. Khalid, et al., Phys. Rev. B 89, 121301(R) (2014).
[5] Y. Yuan, et al.,IEEE Trans. Magn. 50, 2401304 (2014).
[6] M. Khalid, et al., J. Appl. Phys. 117, 043906 (2015).
[7] Y. Yuan, et al., J. Phys. D: Appl. Phys. 48, 235002 (2015).
[8] S. Zhou, J. Phys. D: Appl. Phys. 48, 263001 (2015).
[9] Y. Yuan, et al., ACS Appl. Mater. Interfaces, 8, 3912 (2016).
[10] L. Li, et al., J. Phys. D: Appl. Phys. 44 099501 (2011).
[12] S. Zhou, et al., Phys. Rev. B 94, 075205 (2016).

Primary authors:
Dr. ZHOU, Shengqiang (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Mr. YUAN, Ye (HZDR) Prof. SAWICKI, M. (Institute of Physics, Polish Academy of Sciences, Warszawa, Poland) Dr. RUSHFORTH, A. W. (University of Nottingham, Nottingham NG7 2RD, UK) Prof. ZHAO, Jianhua (Institute of Semiconductors, Chinese Academy of Science, Beijing 100080, China) Prof. TIMM, C. (Technische Universität Dresden, 01062 Dresden, Germany) Prof. HELM, M. (HZDR)

Asymmetric Thermal Lineshape Broadening in the Dimerised Antiferromagnet BaCu2V2O8

Content:

Despite the conventional picture which suggests symmetric Lorentzian broadening of magnetic excitations as temperature is increased, the magnets, where the excitations are strong interact with each other, display the asymmetric thermal lineshape broadening [1,2]. In present work we introduce our investigations of a highly dimerised 1D antiferromagnet BaCu2V2O8 which is a potential candidate for the observation of asymmetric thermal line shape broadening. BaCu2V2O8 has a tetragonal symmetry where the magnetic Cu2+ ions (spin-1/2) form alternating spiral chains along the c-axis. Our inelastic neutron scattering measurements on a single crystal of BaCu2V2O8 reveal that the magnetic excitations consist of two excitation branches, which have a gap of 36meV and disperse along the L direction over the energy range 36-46 meV. Both modes are dispersionless in the H and K directions implying that the dimers are coupled together one-dimensionally along the c-direction, but with negligible coupling within the a-b plane. The high ratio of gap to bandwidth (=3.6) in BaCu2V2O8 make this a candidate compound for detailed observation for asymmetric thermal lineshape broadening over a wide temperature range. The analysis of the high resolution energy scans, which were measured at the dispersion minima at different temperatures, reveals that the line shape becomes asymmetric with increasing temperature which can be attributed to strong correlations between the excitations [3]. These results confirm that excitations in strongly dimerised 1D magnetic systems behave as a 1D strongly correlated gas of Bosons.

[1] D. L. Quintero-Castro, B. Lake, et al Phys. Rev. Lett. 109, 127206 (2012).
[2] D. Tennant, B. Lake, , et al. Phys. Rev. B 85, 014402 (2012).
[3] E. S. Klyushina, A. C. Tiegel, B. Fauseweh, A.T.M.N. Nazmul, J. T. Park, B. Klemke, A. Honecker, G. S. Uhrig, S. R. Manmana, B. Lake. Phys. Rev. B 93, 241109(R) (2016)

Primary authors:
Mrs. KLYUSHINA, Ekaterina (Helmholtz-Zentrum Berlin für Materialien und Energie (HZB))

Co-authors :
Prof. LAKE, Bella (Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)) Dr. ISLAM, Nazmul (Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)) Dr. PARK, Jitae (Technischen Universität Berlin)

Biofilm formation and bacterial stress response studied by X-ray microscopy

Content:

Biofilms are assemblages of bacteria attached to a surface and enclosed in an adhesive matrix of extracellular polymeric substances (EPS) [1]. In this state, the bacteria develop an increased robustness against antimicrobial agents. Biofilms form on most surfaces, e.g., medical devices such as catheters and implants, but also in industrial environments such as food processing plants or in cooling systems. Thus, they are of major concern in medicine and in many commercial enterprises.
In this context it is important to understand the processes that lead to biofilm formation and the mechanisms involved in bacterial stress response.
We investigated the morphology and elemental composition of bacterial aggregates on interfaces by synchrotron radiation-based hard X-ray microscopy techniques. Microtomography experiments with minimum sample preparation using full-field transmission X-ray microscopy (TXM) [2] with Zernike phase contrast were performed on different biofilm-habitat interfaces to explore the three-dimensional organization of the biofilm. Stress response mechanisms including relevant trace elements and their spatial distribution were studied by correlative imaging by hard X-ray phase contrast tomography (holotomography) [3] combined with hard X-ray fluorescence microscopy (SXFM) [4] with tens of nanometers resolution and sub-ppm sensitivity. This complementary information may provide clues about the microbial architectures, the chemical composition of the biofilm matrix and possible molecular functions.

[1] Madigan M.T., Martinko J.M., Stahl D.A., Clark D.P., Brock Biology of Microorganisms, Pearson Press, 2009.
[2] Yin G.C., Tang M.T., Song Y.F., Chen F.R., Liang K.S., Duewer F.W., Yun W., Ko C.H., Shieh H.P.D., Energy-tunable transmission X-ray microscope for differential contrast imaging with near 60 nm resolution tomography., Applied Physics Letters 88, Issue 24, 241115 (2006).
[3] Cloetens, Peter, et al. Hard x-ray phase imaging using simple propagation of a coherent
synchrotron radiation beam. Journal of Physics D: Applied Physics 32, Issue 10A, A145 (1999).
[4] Ortega R, Cloetens P, Devès G, Carmona A, Bohic S, Iron Storage within Dopamine Neurovesicles Revealed by Chemical Nano-Imaging. PLoS ONE 2(9), e925 (2007).

Primary authors:
Dr. HEINE, Ruth (Karlsruhe Insititute of Technology) Dr. YANG, Yang (Karlsruhe Institute of Technology)

Co-authors :
Ms. KIRCHEN, Silke (Karlsruhe Institute of Technology) Ms. DEBASTIANI, Rafaela (Karlsruhe Institute of Technology) Dr. GORNIAK, Thomas (Ruhr-University Bochum) Dr. SENKBEIL, Tobias (Ruhr-University Bochum) Prof. ROSENHAHN, Axel (Ruhr-University Bochum) Dr. XU, Feng (Karlsruhe Institute of Technology) Dr. SUHONEN, Heikki (ESRF) Dr. HELFEN, Lukas (ESRF) Ms. BARTELS, Carolin (University of Heidelberg) Dr. WACKER, Irene (University of Heidelberg) Dr. SONG, Yen-fang (NSRRC, Taiwan) Dr. WANG, Chung-chieh (NSRRC, Taiwan) Prof. GRUNZE, Michael (University of Heidelberg) Prof. SCHWARTZ, Thomas (Karlsruhe Institute of Technology) Prof. BAUMBACH, Tilo (Karlsruhe Institute of Technology)

Bragg coherent x-ray diffractive imaging of a single nanowire

Content:

I will present the work performed at DESY in the framework of RT4, materials and nanoscience for information technology.
The project is dedicated to 2D and 3D studies of strain distribution in a single semiconductor nanowires.
Revealed information allows to establish the link between structural and functional properties of nanowire based devices.

Primary authors:
Mr. DZHIGAEV, Dmitry (DESY)

COMOTION - Controlling the motion of very large molecules and particles

Content:

Recent years saw the development of several techniques to control and confine various degrees of freedom of neutral molecules. We can now routinely select single structural isomers of small molecules, disperse rotational quantum-states, and in certain cases create single-quantum-state samples [1]. These are ideally suited for further manipulation using alignment and orientation techniques [2], allowing experiments to be carried out within the molecular frame of reference.
Thus, direct information on the nuclear and electronic structure can be obtained. Here we report on the COMOTION project, which aims to extend the available techniques to significantly larger systems, from (poly-)peptide molecules to entire cells or viruses.
Using soft vaporisation techniques, such as laser or acoustic desorption, allows the production of large volatile (bio)molecules in the gas-phase. These can subsequently be cooled using supersonic expansions or cryogenic buffer-gas cells. Different approaches are needed for the production of nanoparticle-sized systems. While these can be introduced into the gas-phase using liquid microjet injectors, achieved densities are typically low and particles encased in solvent. We are working on overcoming these issues through the use of aerodynamic lens stacks [3] and convergent-nozzle focusing injectors [4] to produce controlled particle beams. These controlled particle beams can subsequently be manipulated using optical techniques, such as tractor beams or optical pipelines [5,6], to focus particles further and steer them into a well-defined interaction volume. We present first results from our new laser desorption and laser-induced acoustic desorption setups. These have been designed specifically for incorporation into x-ray-free-electronlaser experiments and provide the required experimental flexibility. For aerosol particle injectors we present novel characterisation techniques that allow direct visualisation of the particle and the gas stream, as well as determination of the particle concentration and velocity [7,8]. These tools significantly aid in alignment of tightly focused or collimated particle beams with nano-focused Xray beams in single-particle diffractive imaging experiments. We furthermore report on progress of controlling the translational degrees of freedom of aerosol particles in vacuum using shaped laser beams, working towards an optical funnel for delivering particles with micrometer precision into an interaction region.

[1] Chang, Horke, Trippel, Küpper, Int. Rev. Phys. Chem. 34, 557 (2015)
[2] Trippel, Mullins, Müller, Kienitz, Długołęcki, Küpper, Mol. Phys. 111, 1738 (2013)
[3] Bogan et. al., Aerosol. Sci. Tech. 44, i (2010)
[4] Kirian et. al., Struct. Dyn. 2, 041717 (2015)
[5] Eckerskorn, Li, Kirian, Küpper, DePonte, Krolikowski, Lee, Chapman, Rode, Opt. Expr. 21, 30492 (2013)
[6] Eckerskorn, Bowman, Kirian, Awel, Wiedorn, Küpper, Padgett, Chapman, Rode, Phys. Rev. Appl. 4, 067001 (2015)

[7] Awel, Kirian, Eckerskorn, Wiedorn, Horke, Rode, Küpper, Chapman, Opt. Expr. 24, 6507 (2016)
[8] Horke, Roth, Worbs, Küpper, submitted (2016); arXiv: 1609.09020

Primary authors:
HORKE, Daniel (Center for Free-Electron Laser Science, DESY, Hamburg, Germany)

Co-authors :
()

Charge transfer dynamics in halomethane molecules ionized by intense femtosecond X–ray pulses

Content:

Electron transfer processes induced by photoabsorption play a central role in a broad range of physical, chemical, and biological reactions. Charge transfer phenomena involve electronic as well as nuclear motion and are, therefore, closely related to molecular bond formation and breaking. The microscopic understanding of their dynamics is crucial for emerging photosynthetic, photocatalytic, and photovoltaic applications.

Here, the results of a femtosecond pump–probe experiment conducted at the LCLS free–electron laser are presented, aimed at studying electron transfer dynamics initiated by inner–shell ionization of a halogen atom in gas–phase iodomethane (CH3I) and fluoromethane (CH3F) molecules [1]. Through inner–shell ionization followed by (local) Auger decay, multiple charges can be induced with a high degree of spatial localization at a heavy element with a large X–ray absorption cross section. The subsequent electron dynamics are strongly influenced by the initial positions of the nuclei, and by the interplay between electronic and nuclear motion. Depending on the internuclear distance at the time of the X–ray absorption, the charge either remains on the absorbing halogen or spreads over to the molecular environment. By measuring the charge state and the kinetic energy distributions of the created ionic fragments, the charge rearrangement between the two molecular centers can be traced as a function of their internuclear separation.

Iodomethane can be efficiently broken up into two neutral fragments, and its UV–induced photolysis in the A band is a prototypical photodissociation process which is well studied experimentally and theoretically. Fluoromethane is known to exhibit intriguing electron transfer dynamics upon fluorine (1s) photoabsorption, and fluorine as the most electronegative element is a predestined candidate to initiate charge transfer to the molecular environment. The experimental results are complementary, due to the qualitatively different reactions of the two species to UV irradiation, as well as the considerably different electronegativities of the two halogen atoms.

Signatures of long–distance intramolecular charge transfer are observed for both molecules, and a quantitative analysis of its distance dependence in iodomethane is carried out for charge states up to I21+. The reconstructed critical distances for electron transfer are in good agreement with a classical over–the–barrier model and with an earlier experiment employing a near–infrared pump pulse [2]. Combined with coincident electron spectroscopy and upcoming attosecond soft X–ray pulses, this approach will allow tracing local charge propagation dynamics with Angstrom spatial and sub–femtosecond temporal resolution.

References

[1] R. Boll, B. Erk, R. Coffee, S. Trippel, T. Kierspel, C. Bomme, J. D. Bozek, M. Burkett, S. Carron, K. R. Ferguson, L. Foucar, J. K¨upper, T. Marchenko, C. Miron, M. Patanen, T. Osipov, S. Schorb, M. Simon, M. Swiggers, S. Techert, K. Ueda, C. Bostedt, D. Rolles, and A. Rudenko, Charge transfer in dissociating iodomethane and fluoromethane molecules ionized by intense femtosecond X–ray pulses, Struct. Dyn. 3, 043207 (2016).

[2] B. Erk, R. Boll, S. Trippel, D. Anielski, L. Foucar, B. Rudek, S. W. Epp, R. Coffee, S. Carron, S. Schorb, K. R. Ferguson, M. Swiggers, J. D. Bozek, M. Simon, T. Marchenko, J. K¨upper, I. Schlichting, J. Ullrich, C. Bostedt, D. Rolles, and A. Rudenko, Imaging charge transfer in iodomethane upon x-ray photoabsorption, Science 345, 288 (2014).

Primary authors:
BOLL, Rebecca (DESY, Hamburg)

Chirality induced exchange bias effect in DyCo/FeNi bilayers

Content:

Keywords: polarized neutron reflectometry, polarization analysis, chirality, exchange bias

Alloys of rare-earth elements and 3d transition metals became recently again in the focus of attention due there rich variety of magnetic effects owed to the different anisotropies of both material classes [1-4].
In this work, a dual in-plane exchange bias effects (HEB=±39mTesla) were found in the orthogonal coupled thin Dy20Co80/NiFe bilayer occurring at room temperature without the need of any field cooling procedure. Particularly interesting, the direction of the exchange bias effect can be switched by changing solely the direction of the perpendicular magnetic fields in relative moderate fields of about 200mT. The in-plane exchange bias keeps stable even at extern in-plane magnetic fields of more than 6T. The underlying mechanism behind the extraordinary effect was investigated with magnetic optical Kerr effect (MOKE), X-ray magnetic circular dichroism (XMCD) and polarized neutron reflectometry measurements (PNR). Particularly the use of polarized neutrons enabling one to get access to the chemical and magnetic depth profile was essential to identify chirality as the crucial mechanism behind the intriguing isothermal exchange bias effect. The application of polarization analysis allowed us to analyze the non-collinear magnetic structure during the switching behavior in detail. The exchange bias in NiFe can be attributed to the interface exchange coupling to the DyCo layer, while the exchange bias in DyCo layer is due to the formation of chirality in its spin structure formed during the deposition on NiFe. Latter indicates a Dyzaloshinskii-Moriya like term in the interacting energy originating from the broken inversion symmetry at the interface between both magnetic layers. Such chirality based exchange bias systems may be of crucial importance for the development of future applications in the field of magnetic sensors.

[1] S. Mangin et.al, Phys. Rev. B 80, 224424 (2009), S. Mangin et.al, Phys. Rev. Lett. 82, 4336 (1999)
[2] Chen, K., Lott, D. et al.. Phys. Rev. B 91, 024409 (2015)
[3] Chen, K., Lott, D. et al., Sci. Rep. 5, 18377 (2015);
[4] F. Radu, R. Abrudan, I. Radu, D. Schmitz, H. Zabel, Nat. Communications 3, 715 (2012).

Primary authors:
LOTT, Dieter (Institute for Materials Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany)

Co-authors :
CHEN, Kai (Institute of Physics II, University of Cologne, Zülpicher Straße 77, D-50937 Cologne, Germany) LAUTER, Valeria (Spallation Neutron Source, Oak Ridge National Laboratory, USA)

Code de Vita

Content:

We provide an overview on a project which optimizes dose in propagation based X-ray imaging of living and fixed organisms in a parallel beam using (i) a set-up employing Bragg magnification plus single-photon counting detectors and (ii) indirect detection with visible-light optics.

Primary authors:
Dr. HOFMANN, Ralf (IPS)

Co-authors :
BAUMBACH, Tilo (IPS, KIT)

Coherent diffraction nanocatalysis

Content:

The nanoparticle shape is an influential factor in many catalytic activities because it could dictate the adsorption free energy by the atomic arrangement on the catalyst surface[1]. Therefore, in order to understand the size-dependence of catalytic processes novel approaches to controlled nanocatalysis are required[2].

In this work we report on a one-to-one structure analysis of randomly deposited Ir nanodots, a single Pt nanodot and a single Pt nanodot-array, all of them epitaxially grown on STO(100) single crystals[3]. We aim to understand the atomic structure and shape of these nanoparticles during catalytic CO oxidation under continuous flow at near ambient pressures by in-situ coherent Bragg diffraction using a nanofocused X-ray beam at a 3rd generation synchrotron source.

The nanoparticles were pre-selected by SEM, marked by FIB and characterized by AFM, providing real space structural information, and in reciprocal space under static and in-situ conditions using coherent Bragg diffraction[4] from a focused X-ray beam at PETRA III and ESRF, utilizing a transfer and repositioning protocol using the Pt X-ray fluorescence. The Pt nanodot-array was created by top-down nanofabrication process using a combined lift-off and etching methods based on e-beam lithography, whereas the Ir nanodots were deposited by e-beam evaporation[5].

This in-situ study will give first insights into the structure, faceting and growth of these nanoparticles and their mutual nanoscale interaction under catalytic CO oxidation conditions. We expect that our experiment will facilitate and stimulate future experiments on in-situ oxidation or catalysis of single nano-objects exploiting coherent X-ray diffraction and imaging (CDI) under reaction conditions.

REFERENCES
1. Strmcnik DS, Tripkovic DV, Van Der Vliet D, Chang KC, Komanicky V, You H, Karapetrov G, Greeley JP, Stamenkovic VR, Marković NM, J Am Chem Soc 130, 15332–15339 (2008).
2. Komanicky V, Iddir H, Chang KC, Menzel A, Karapetrov G, Hennessy D, Zapol P, You H, J Am Chem Soc 131, 5732–5733 (2009).
3. Komanicky, V.; Iddir, H.; Chang, K. C.; Menzel, A.; Karapetrov, G.; Hennessy, D. C.; Zapol, P.; You, H. Electrochim. Acta 55, 7934–7938 (2010).
4. Huang, W. J.; Sun, R.; Tao, J.; Menard, L. D.; Nuzzo, R. G.; Zuo, J. M. Nat. Mater. 7, 308–313 (2008).
5. Schülli, T.; Trenkler, J.; Mönch, I.; Bolloc'h, D. Le; Dosch, H. Europhys. Lett. 58, 737–743 (2002).

Primary authors:
Dr. ABUíN, Manuel (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany)

Co-authors :
Dr. KELLER, Thomas F. (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany. Institute for Nanostructure and Solid State Physics, University of Hamburg, Germany) Dr. SHAYDUK, Roman (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. VONK, Vedran (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. DANGWAL PANDEY, Arti (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. NEISSER, Claudia (Institute for Ion Beam Physics, Helmholtz Center Dresden-Rossendorf, Germany) Dr. KIM, Young Yong (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. DZHIGAEV, Dmitry (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. LAZAREV, Sergey (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. VARTANIANTS, Ivan (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany) Dr. STIERLE, Andreas (Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany)

Coincidence imaging of molecules with a high-photon-flux high-harmonic source

Content:

The talk will report on the recent developments in high-photon-flux high-harmonic sources. In addition, first experiments on inner-shell excitation of iodomethane molecules and subsequent fragment detection in coincidence have been performed. In future, time-resolved experiments with femtosecond and attosecond precision will be feasible.

Primary authors:
Dr. ROTHHARDT, Jan (Helmtoltz Institute Jena)

Combining the strengths of Neutrons and Molecular dynamics for the study of bio-membranes

Content:

Neutron reflectometry is one of the most powerful methods for investigating the structure of model lipid membranes. These model systems are more easily prepared and experimentally controlled than natural lipid membranes, which are an important integral part of animal and plant cells. In the present work we combine measurements of supported lipid membranes (SLBs) at the MARIA neutron reflectometer and coarse-grained molecular dynamics simulations using the MARTINI force field, for the precise characterization of SLBs at the sub-nanometer scale. The proposed methodology delivers more precise results and should pave the way for studying membranes of a more complex nature, having in mind experiments where membranes interact with bio-molecules, e.g. proteins, small peptides, and nanoparticles that are candidates for drug delivery applications.

Primary authors:
KOUTSIOUMPAS (Jülich Centre for Neutron Science (JCNS))

Comprehensive in situ processing and characterization of nanocomposite materials

Content:

The detailed knowledge of composition and microstructure is essential for the understanding of processes and properties of nanocomposite materials for applications at high temperatures. To ensure materials functionality under in operando conditions, new concepts for analysis and process monitoring are necessary. In this contribution, selected PVD deposited thin film material systems were studied in situ at temperatures up to 830°C by Rutherford backscattering spectrometry (RBS), Raman spectroscopy, and spectroscopic ellipsometry (SE) within a cluster tool.

Metal-induced crystallization with and without layer exchange (MIC w/o LE) is an emerging technique for processing of amorphous group 14 elements below their isothermal crystallization temperature. As model system, a bilayer of 60 nm amorphous Si covered by 30 nm Ag (a-Si/Ag) was deposited in situ and studied at temperatures of 380 to 700°C by the combination of the above-listed techniques. More than 90% of the initial a-Si could be crystallized on top of the Ag-layer for optimized process conditions. The as-formed Si consisted of up to 95% crystalline Si.

As example for high-temperature solar-selective coatings for thermo-solar applications, AlTiN and AlTiN1-xOx (x = 0 - 0.2) thin films were investigated in order to understand the influence of the oxygen/nitrogen ratio on the optical properties and failure mechanisms at high temperatures. The elemental depth profiles and the phase structure of both coatings do not change during annealing in high vacuum at temperatures up to of 750°C, as revealed by unchanged RBS and Raman spectra, respectively. SE and RBS results showed the influence of the initial oxygen content on high temperature stability of AlTiN and AlTiN1-xOx thin films. The low emittance of AlTiN1-xOx, allowed performing in situ RBS analysis at temperatures up to 830°C for the first time.

Financial support by the EU, grant No. 645725, project FRIENDS2, and the HGF via the W3 program (S.G.) is gratefully acknowledged.

Primary authors:
Dr. KRAUSE, Matthias (Helmholtz-Zentrum Dresden - Rossendorf)

Co-authors :
WENISCH, Robert (Helmholtz-Zentrum Dresden - Rossendorf) JANKE, Daniel (Helmholtz-Zentrum Dresden - Rossendorf) Dr. HERAS, Irene (Abengoa Research S.L., Seville, Spain) LUNGWITZ, Frank (Helmholtz-Zentrum Dresden - Rossendorf) Dr. GUILLéN, Elena (Abengoa Research S.L., Seville, Spain) Dr. HELLER, Rene (Helmholtz-Zentrum Dresden - Rossendorf) Dr. ESCOBAR GALINDO, Ramon (Abengoa Research S.L., Seville, Spain) Dr. GEMMING, Sibylle (Helmholtz-Zentrum Dresden - Rossendorf and TU Chemnitz)

Constructing nanoelectronic circuits by top-down and bottom-up strategies

Content:

The construction of nanoelectronic circuits requires the development of bottom-up strategies, which can be combined with top-down structuring. As a typical example for top-down structuring, we show how reconfigurable silicon nanowires are produced using electron-beam lithography and reactive ion etching. Such structures can be used as large-scale electrodes to networks of self-assembled electronics on the nanoscale. As a first step towards the development of nanoscale circuits by self-organization, we demonstrate the construction of nanoscale metallic wires based on metallized DNA origamis [1]. Active building blocks with smallest dimensions on the molecular scale are developed in single molecule contacts. The properties of those junctions need to be characterized. We have demonstrated that the mechanically controllable break junction (MCBJ) technique can be successfully used to determine the properties of electronic transport through single organic molecules and that the participating molecular energy levels and the metal-molecule coupling can be characterized using this technique [2]. Further developments are based on the use of more complex molecules, which can, for example, be used as single molecule switches [3][4]. We present the first demonstration of a single molecule junction, in which the molecule is switched in situ from the non-conducting “off”-state to the conducting “on”-state.

References

1. Teschome, B. et al. Temperature-Dependent Charge Transport through Individually Contacted DNA Origami-Based Au Nanowires. Langmuir 32, 10159–10165 (2016).

2. Zotti, L. A. et al. Revealing the Role of Anchoring Groups in the Electrical Conduction Through Single-Molecule Junctions. Small 6, 1529–1535 (2010).

3. Sendler, T., Guth, K. L., Wieser, M. & Wolf, J. Light-Induced Switching of Tunable Single-Molecule Junctions. Advanced … (2015). doi:10.1002/advs.201500017

4. Kim, Y. et al. Charge Transport Characteristics of Diarylethene Photoswitching Single-Molecule Junctions. Nano Lett 120628135846000 (2012). doi:10.1021/nl3015523

Primary authors:
Mr. KILIBARDA, Filip (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Dr. SENDLER, Torsten (Helmholtz-Zentrum Dresden-Rossendorf) Mr. DEB, Dipjyoti (Helmholtz-Zentrum Dresden-Rossendorf) Mr. KHAN, Muhammad Bilal (Helmholtz-Zentrum Dresden-Rossendorf) Mr. TESCHOME, Bezu (Helmholtz-Zentrum Dresden-Rossendorf) Dr. ERBE, Artur (Helmholtz-Zentrum Dresden-Rossendorf)

Controlling the Dzyaloshinskii-Moriya interaction to alter the chiral link between structure and magnetism

Content:

The cubic B20 compounds have a non-centrosymmetric crystallographic structure described by the P213 space group. The lack of a symmetry center of the crystal structure produces a chiral Dzyaloshinskii-Moriya (DM) interaction, resulting in the appearance of a spin helix with a certain chirality □m [1,2]. The sense of the magnetic chirality □m is rigorously determined by the sense of the crystalline chirality (see for example [3]). Our recent small angle neutron scattering investigations of the monogermanide based compounds Mn1-xFexGe[3] and Fe1-yCoyGe [4] suggest a flip of the chiral link between structural and magnetic chirality in these compounds at a critical concentration xc,yc. The change of the sign of the product of □c x □m goes along with the transformation of the spiral to a ferromagnetic spin structure caused by the cubic anisotropy [5]. In this work, we will present the possibility to gain full control of the DM interaction by means of the single crystalline Fe1-zCozSi compounds [6]. Using the Czochralski technique the structural chirality of the produced Fe1-zCozSi samples could be controlled by nearly 100% [7]. We synthesized Fe1-zCozSi with z = 0.5, 0.6, 0.65, 0.7 and 0.8. The determination of the absolute structure by single crystal x-ray diffraction at the PILATUS@SNBL diffractometer at the BM01A end station at the Swiss-Norwegian Beamline at the ESRF (Grenoble, France) confirms the right handed structural chirality for all investigated samples. The helix wave vector ks, as extracted from the low temperature neutron scattering maps, show a critical behavior for zc = 0.65. The single crystal nature of the samples allows the direct determination of the magnetic chirality using polarized small angle scattering. The polarized neutron measurements (performed at the SANS-1 instrument at the Heinz-Maier Leibnitz Zentrum in Garching, Germany) confirm the flip of the chiral link between structural and magnetic chirality for z < zc and z > zc.
In summary, we show the proof of concept to apply the DMI to gain full control of the magnetic chirality in cubic B20 helimagnets and, furthermore, give the experimental evidence for the important role of the cubic anisotropy in these systems.

[1] P. Bak and M.H. Jensen, J. Phys. C13, L881 (1980).
[2] O. Nakanishi, et al., Solid State Commun. 35, 995-998 (1980).
[3] S.V. Grigoriev et al., Phys. Rev. Lett. 110, 207201 (2013).
[4] S.V. Grigoriev, et al., Phys. Rev. B 90, 174414 (2014).
[5] S.V. Grigoriev, et al., Phys. Rev. B 91, 224429 (2015).
[6] S.-A. Siegfried, et al., Phys. Rev. B 91, 184406 (2015).
[7] V.A. Dyadkin, et al., Phys. Rev. B 84, 014435 (2011).

Primary authors:
SIEGFRIED, Sven-arne (Helmholtz-Zentrum Geesthacht, Geesthacht, 21502, Germany)

Co-authors :
ALTYNBAEV, Evgeny V. (Petersburg Nuclear Physics Institute, Gatchina, 188300 St-Petersburg, Russia and Faculty of Physics, Saint-Petersburg State University, 198504 St-Petersburg, Russia) CHUBOVA, Nadya M. (Petersburg Nuclear Physics Institute, Gatchina, 188300 St-Petersburg, Russia) DYADKIN, Vadim A. (Swiss-Norwegian Beamlines at the ESRF, Grenoble Cedex, 38043 France and Petersburg Nuclear Physics Institute, Gatchina, 188300 St-Petersburg, Russia) CHERNYSHOV, Dimitry (Swiss-Norwegian Beamlines at the ESRF, Grenoble Cedex, 38043 France) MOSKVIN, Evgeny V. (Petersburg Nuclear Physics Institute, Gatchina, 188300 St-Petersburg, Russia and Faculty of Physics, Saint-Petersburg State University, 198504 St-Petersburg, Russia) MENZEL, Dirk (Technische Universität Braunschweig, Braunschweig, 38106, Germany) HEINEMANN, André (Helmholtz-Zentrum Geesthacht, Geesthacht, 21502, Germany) SCHREYER, Andreas (European Spallation Source ERIC, P.O. Box 176, SE-221 00 Lund, Sweden) GRIGORIEV, Sergey V. (Petersburg Nuclear Physics Institute, Gatchina, 188300 St-Petersburg, Russia and Faculty of Physics, Saint-Petersburg State University, 198504 St-Petersburg, Russia)

Coupled charge density wave and magnetism in TbTe3

Content:

Superconductivity (SC) and charge-density-waves (CDW) are collective electronic phenomena that originate from electron-electron and electron-phonon interactions, and the concept of Fermi surface competition between these collective states is one of the most fundamental problems of condensed matter physics. Some of the systems that exhibit such an interplay of SC and CDW (ex: layered transition-metal chalcogenides, and the copper-oxide high-Tc superconductors) also develop complex magnetic orders and a delicate interplay between the different phases is revealed as a function of temperature, pressure and magnetic field. Another example is TbTe3 which displays a rich combination of quantum cooperative phenomenon including 2 charge density wave orders, complex incommensurate and commensurate magnetic orders as well as unconventional superconductivity. In this work we have studied the interplay of the CDW and magnetic orders in TbTe3 as a function of temperature and magnetic field. We find that these two states coexist at all the temperatures below the magnetic transition and that the magnetic order is coupled to the CDW state such that the magnetic wave vector can be described in terms of the CDW wave vector. Furthermore, we find an additional field induced phase where, the wave vector corresponding to magnetic order locks-in to the CDW wave vector. Therefore, TbTe3 can be considered as an ideal system to study the coexistence of magnetism and CDW orders.

Primary authors:
Dr. CHILLAL, Shravani (Helmholtz Zentrum Berlin)

Co-authors :
Prof. LAKE, Bella (Helmholtz Zentrum Berlin) Dr. SCHIERLE, Enrico (Helmholtz Zentrum Berlin) Dr. YOKAICHIYA, Fabiano (Helmholtz Zentrum Berlin) Dr. HOFFMANN, Jens U (Helmholtz Zentrum Berlin) Dr. VASSILIEV, Alexandre (M.V. Lomonosov Moscow State University) Dr. VOLKOVA, Olga (M.V. Lomonosov Moscow State University) Dr. MONCEAU, Pierre (Universite Grenoble Alpes, Institut Neel) Dr. WESCHKE, Eugen (Helmholtz Zentrum Berlin)

Curved Magnetic Nanomembranes

Content:

While conventionally magnetic films and structures are fabricated on flat surfaces, the topology of curved surfaces has only recently started to be explored and leads to new fundamental physics as well as applied device ideas [1]. In particular, novel effects occur when the magnetization is modulated by curvature providing a new degree of freedom that leads to new magnetization configurations (see for instance [2,3]) and is predicted to have major implications on the spin dynamics due to topological constraints for instance in circular tubes and rolls [4].

Advances in this novel field solely rely on the understanding of the fundamentals behind the modifications of magnetic responses of 3D-curved magnetic thin films. The lack of an inversion symmetry and the emergence of a curvature induced effective anisotropy and Dzyaloshinskii-Moriya interaction are characteristic of curved surfaces [5-7], leading to curvature-driven magnetochiral effects [8-10] and topologically induced magnetization patterning [7, 11], including unlimited domain wall velocities in hollow tubes [4], chirality symmetry breaking [7-10] and Cherenkov-like effects for magnons [12]. In addition to these rich physics, the application potential of 3D-shaped objects is currently being explored as magnetic field sensorics for magnetofluidic applications [13], spin-wave filters [14], magneto-encephalography devices [15] and high-speed racetrack memory devices [4]. To this end, the initially fundamental topic of the magnetism in curved geometries strongly benefited from the input of the application-oriented community, which among others explores the shapeability aspect of the curved magnetic thin films. These activities resulted in the development of the family of shapeable magnetoelectronics [16], which already includes flexible [17], printable [18], stretchable [19] and even imperceptible [20] magnetic field sensorics.

These recent developments starting from the theoretical predictions to the fabrication and characterization of 3D-curved magnetic thin films and their application potential are in the focus of this presentation.

References

[1] R. Streubel, DM et al., J. Phys. D: Appl. Phys. vol. 49, pp. 363001, 2016.
[4] M. Yan et al., Phys. Rev. Lett. vol. 104, pp. 057201, 2010.
[5] Y. Gaididei et al., Phys. Rev. Lett. vol. 112, pp. 257203, 2014.
[6] O. V. Pylypovskyi, DM et al., Phys. Rev. Lett. vol. 114, pp. 197204, 2015.
[7] O. V. Pylypovskyi, DM et al., Sci. Rep. vol. 6, pp. 23316, 2016.
[8] R. Hertel, SPIN vol. 03, pp. 1340009, 2013.
[9] M. Yan et al., Appl. Phys. Lett. vol. 100, pp. 252401, 2012.
[10] J. A. Otalora et al., Appl. Phys. Lett. vol. 100, pp. 072407, 2012.
[11] V. P. Kravchuk, DM et al., Phys. Rev. B vol. 85, pp. 144433, 2012.
[12] M. Yan et al., Phys. Rev. B vol. 88, pp. 220412, 2013.
[13] I. Mönch, DM et al., ACS Nano vol. 5, pp. 7436, 2011.
[14] F. Balhorn et al., Phys. Rev. Lett. vol. 104, pp. 037205, 2010.
[15] D. Karnaushenko, DM et al., Adv. Mater. vol. 27, pp. 6582, 2015.
[16] D. Makarov et al., Appl. Phys. Rev. vol. 3, pp. 011101, 2016.
[17] M. Melzer, DM et al., Adv. Mater. vol. 27, pp. 1274, 2015.
[18] D. Karnaushenko, DM et al., Adv. Mater. vol. 27, pp. 880, 2015.
[19] M. Melzer, DM et al., Nano Lett. vol. 11, pp. 2522, 2011.
[20] M. Melzer, DM et al., Nature Commun. vol. 6, pp. 6080, 2015.

Primary authors:
Dr. MAKAROV, Denys (Helmholtz-Zentrum Dresden-Rossendorf e.V.)

Co-authors :
Dr. VOLKOV, Oleksii (Helmholtz-Zentrum Dresden-Rossendorf e.V.) Prof. FASSBENDER, Jürgen (Helmholtz-Zentrum Dresden-Rossendorf e.V.)

Custom-Made Magneto-Resistive Multilayer Devices

Content:

A free adjustment of magnetoresistive sensor characteristics in arbitrary magnetic/nonmagnetic multilayer stacks is achieved via sputter deposition at oblique incidence. The approach allows to precisely set the magnetization axis and switching field of each individual layer via the polar and azimuthal angle of deposition.
Newly accessible multilayer spin structures form the basis for advanced, custom-made magnetoresistive sensor applications and multiple addressable remanent states might be advantageous for new magnetic memory applications.

Primary authors:
Dr. SCHLAGE, Kai (DESY)

Co-authors :
Dr. BOCKLAGE, Lars (DESY) Dr. ERB, Denise (DESY) Ms. COMFORT, Jade (DESY) Dr. WILLE, Hans-christian (DESY) Prof. ROEHLSBERGER, Ralf (DESY)

Defect-free accommodation of strain in highly mismatched GaAs/InxGa1-xAs core/shell nanowires

Content:

The nanowire (NW) geometry enables the pseudomorphic growth of highly mismatched semiconductor heterostructures beyond the critical thickness of their thin film counterparts. In this work, we have investigated the mismatch strain in free-standing GaAs/(In,Ga)As core/shell NWs, which were grown on Si (111) by molecular beam epitaxy. The NWs have a zinc blende structure with their axis along the [111] crystallographic direction, and six {11$\bar{2}$0} sidewalls. Our study focused explicitly on NWs with a core diameter as small as 25 nm. For the analysis of the strain, we used Raman scattering spectroscopy, transmission electron microscopy (TEM) and X-ray diffraction (XRD), and compared the results with theoretical simulations based on continuum elasticity theory and density functional theory. Measuring the shift of the phonon peaks in Raman spectra as a function of the shell thickness (Ls) for a given shell composition (In0.18Ga0.82As), the strain state of the core and the shell could be determined. That is, the core is under tensile hydrostatic stress that increases with Ls and saturates for Ls > 20 nm. On the other hand, the shell is under compressive stress that decreases with Ls and almost vanishes for Ls > 20 nm. The strain analysis by Raman is also supported by other findings, like the absence of misfit dislocations along the [11$\bar{2}$] direction of the core/shell interface in high-resolution TEM, or the lattice spacing of the (111) and the (20$\bar{2}$) shell crystal planes in high-resolution XRD. Besides the defect-free accommodation of strain in highly mismatched core/shell NWs, our work demonstrates the unique possibility to confine the elastic energy exclusively inside the core, allowing for the shell to be strain-free.

Primary authors:
Mrs. BALAGHI, Leila (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany, Center For Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany)

Co-authors :
Dr. HüBNER, René (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Dr. BUSSONE, Genziana (PETRA III , Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany) Mr. GRIFONE, Raphael (PETRA III , Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany) Dr. GHORBANI, Mahdi (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Dr. KRASHENINNIKOV, Arkady (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Dr. HLAWACEK, Gregor (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Dr. SCHNEIDER, Harald (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Prof. HELM, Manfred (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany, Center For Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany) Dr. DIMAKIS, Emmanouil (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany)

Direct measurements of the magnetocaloric effect in pulsed magnetic fields

Content:

In the last years big efforts have been made to develop environmental-friendly techniques. The magnetic refrigeration, based on the magnetocaloric effect (MCE), has initiated intensive research activity as a potential candidate to replace the conventional gas compression/expansion technique for cooling applications. A key element on the research on magnetic refrigeration is the development of the suitable materials that exhibit a large MCE and fulfil the conditions to be used in applications. Therefore, the appropriate characterization of the MCE on these materials is fundamental. At the HLD we have developed a technique to measure the MCE under magnetic fields up to 50 T. A brief introduction on the MCE, the technique and important results will be presented.
This work was made in collaboration with M. Ghorbani-Zavareh, C. Felser, O. Gutfleisch, K. Skokov.

Primary authors:
Dr. SALAZAR MEJIA, Catalina (Dresden High Magnetic Field Laboratory)

Co-authors :
Dr. SCURSCHII, Iurii (Dresden High Magnetic Field Laboratory) Prof. WOSNITZA, Jochen (Dresden High Magnetic Field Laboratory)

Drivers of charge dynamics and symmetry breaking in photo-excited Ferricyanide

Content:

The interplay of structural and electronic degrees of freedom are the determining factors in
chemical reactions such as isomerization, dissociation and charge separation processes. We
study $Fe(CN)_6^{3-}$ as a model compound for understanding the mechanisms responsible for
charge propagation and their relation to structural distortions. With resonant inelastic x-ray
scattering (RIXS) at 3d metal L-edges being highly selective to gerade and ungerade valence
states, we are able to directly correlate the appearance and disappearance of spectral
features to symmetry and its breaking. Thereby, we can identify fingerprints of structural
excitations that are the direct result of electronic relaxation mechanisms

Primary authors:
JAY, Raphael M. (Institute for Methods and Instrumentation for Synchrotron Radiation Research, Helmholtz- Zentrum Berlin für Materialien und Energie GmbH, Institut für Physik und Astronomie, Universität Potsdam)

Effect of Base Metal Texture on the Microstructure, Tensile Properties and Residual Stresses of Laser-Welded Titanium Joints

Content:

Single crystals show in general anisotropy in certain properties, such as Young’s modulus, thermal expansion and thermal conductivity, in particular for non-cubic materials. Therefore, the given crystallographic texture affects the properties of polycrystalline material. This can have consequences for the microstructure, mechanical properties and residual stress state of welded joints. In the present work, this influence has been investigated for the case of laser-welded titanium sheet material.
Commercially pure rolled titanium sheets were laser welded using an 8 kW fiber laser at 4 kW laser power with the weld line along rolling direction (RD), transverse direction (TD) and 45° to RD. The three-dimensional strain profile and the local texture around the weld were measured by neutron diffraction at the materials science diffractometer STRESS-SPEC of the Heinz Maier-Leibnitz Zentrum (MLZ). Furthermore, grain orientation within the base material, the heat-affected zone and the fusion zone was investigated using the electron back-scatter diffraction (EBSD) technique. Tensile testing was performed at room temperature on flat tensile samples cut transversely across the weld. The results revealed that the tensile properties differ in various welded sheets having different volume fractions of grains with a certain orientation with respect to the welding direction, while no pronounced texture effect on the residual stress state was observed. In addition, finer grains in the heat affected zone were developed on a joint side where the RD is parallel to the welding direction.

Primary authors:
Dr. MAAWAD, Emad (Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. GAN, Weimin (Helmholtz-Zentrum Geesthacht) Dr. HOFMANN, Michael (Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München) Dr. VENTZKE, Volker (Helmholtz-Zentrum Geesthacht) Mr. RIEKEHR, Stefan (Helmholtz-Zentrum Geesthacht) Dr. KASHAEV, Nikolai (Helmholtz-Zentrum Geesthacht) Prof. MüLLER, Martin (Helmholtz-Zentrum Geesthacht) Prof. BROKMEIER, Heinz-günter (, Clausthal University of Technology)

Efficient multi-cycle terahertz generation in periodically poled crystals by optimized pulse formats

Content:

The generation of high energy, high peak-power and multi-cycle terahertz pulses by using laser pulse sequence in periodically poled lithium niobate and difference frequency generation is studied. Multiple pulse sequence formats are proposed and analyzed. Design strategies to achieve percent level optical-to-terahertz conversion are discussed. Numerical calculations account for nonlinear effects including DFG, SPM, cascaded SHG and damage. The terahertz generation is in the depleted, high conversion regime.

Primary authors:
Dr. BARRE, Damian (CFEL, DESY)

Co-authors :
RAVI, Koustuban (CFEL, DESY) KäRTNER, Rave (CFEL, DESY)

Electronic, Magnetic, and Vibrational properties of Iridates studied via Nuclear Resonant Scattering

Content:

We report on the first observation of nuclear forward scattering (NFS) of synchrotron radiation on the 193-Ir resonance at the energy as high as 73 keV. Following this observation, hyperfine parameters including electric field gradient and the magnetic hyperfine field on the Ir nucleus have been measured in the Ruddlesden-Popper series of strontium iridates for the first time by NFS.
We show that the large penetration depth of 73 keV photons, high natural abundance of 193-Ir (62.7% [1]), and polarization dependence of NFS [1] provide unique possibilities for studies of non-trivial physics in 5d-transition metal oxides. Additionally, we show for the first time the room temperature Mössbauer spectroscopy on Ir metal. This feature is regarded to the high brilliance of the synchrotron radiation source.

References
[1] R. Röhlsberger, Springer Tracts in Modern Physics, Vol. 208, Springer (2004); doi: 10.1007/b86125

Primary authors:
Mr. ALEXEEV, Pavel (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany)

Co-authors :
Dr. WILLE, Hans-christian (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany) Dr. LEUPOLD, Olaf (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany) Dr. SERGUEEV, Ilya (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany) Dr. HERLITSCHKE, Marcus (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany) Prof. RöHLSBERGER, Ralf (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg Germany) Prof. MCMORROW, Desmond F. (London Centre for Nanoscience and Department of Physics and Astronomy, University College London, WC1E 6BT, London, United Kingdom)

Elucidation of LBG polymer film orientation and structure by NEXAFS and calculation by DFT

Content:

Near Edge X-ray Absorption Fine Structure (NEXAFS) has been used to investigate the orientation of various polymers in thin films. The polymers are examples of Low Band Gap (LBG) materials and are important candidates for improving the efficiency of donor-acceptor based bulk hetero junction (BHJ) organic solar cells. The morphology and ability for self-organisation of these materials in thin films strongly influence the properties of the solar cell. NEXAFS is particularly useful in this respect giving both information about the orientation and also the electronic structure. We have used the technique at the Sulphur K edge to study the orientation in films and PCBM blends; the influence of additional (hexyl-)thiophene moieties on film growth and self-organisation and the effect of changing the processing conditions (e.g. [1-3]). Whilst a visual and (semi-)empirical peak fitting approach is useful as first approach calculations and fitting of the data using Density Functional Theory (DFT) allows a better understanding of the transitions and a more detailed analysis of the spectra [4].

[1] U. Aygül, D.R. Batchelor, U. Dettinger, S. Yilmaz, S. Allard, U. Scherf, H. Peisert, T. Chassé, J. Phys. Chem. C 114 (2012) 4870–4874, http://dx.doi.org/10.1021/jp205653n.
[2] U. Aygül, H. Peisert, D.R. Batchelor, U. Dettinger, M. Ivanovic, A. Tournebize, S. Mangold, M. Forster, I. Dumsch, S. Kowalski, S. Allard, U. Scherf, T. Chassé, Sol. Energ. Mat. Sol. Cells. 128 (2014) 119–125, http://dx.doi.org/10.1016/j.solmat.2014.05.017.
[3] M. Ivanovic, U. Aygül, U. Dettinger, A. Tournebize, M. Polek, D.R. Batchelor, S. Mangold, M. Forster, H. Peisert, U. Scherf, T. Chassé, Sol. Energ. Mat. Sol. Cells. 157 (2016) 286–294, http://dx.doi.org/10.1016/j.solmat.2016.05.055.
[4] D.R. Batchelor, U. Aygül, U. Dettinger, M. Ivanovic, A. Tournebize, S. Mangold, M. Forster, H. Peisert, U. Scherf, T. Chassé, Sol. Energ. Mat. Sol. Cells. 157 (2016) 286–294, http://dx.doi.org/10.1016/j.solmat.2016.05.055.

Primary authors:
Dr. BATCHELOR, David (Karlsruhe Insitute of Technology (IPS))

Co-authors :
Dr. AYGÜL, Umut (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany) Mr. IVANOVIC, Milutin (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany) Dr. DETTINGER, Ulf (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany) Dr. TOURNEBIZE, Aurelien (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany) Dr. MANGOLD, Stefan (Karlsruhe Insitute of Technology (IPS)) Dr. FORSTER, Michael (Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Germany) Prof. SCHERF, Ullrich (Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Germany) Dr. PEISERT, Heiko (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany) Prof. CHASSE, Thomas (Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany)

Epitaxial ultra small iron nanoparticle superlattice on graphene on iridium

Content:

Iridium seeding on graphene on Ir(111) allows to epitaxially grow large area ultra small iron nanoparticle superlattices [1]. These are studied with various measurement technics to gain and correlate structural, electronic and magnetic information. The reproducible bottom up process not only enables to compare different samples with LEED, STM, AFM, AES, XPS, but will also make atomically resolved XRD possible [2]. These results will be linked to elaborated magnetic measurements enabled by thin film substrates [3] and capping layers.

[1] – A. T. N'Diaye, et al, New Journal of Physics 11, 103045 (2009)
[2] – D. Franz, et al, Phys. Rev. B 93, 045426 (2016)
[3] – A. Dangwal Pandey, K. Krausert, et al, J. Appl. Phys. 120, 075304 (2016)

Primary authors:
KRAUSERT, Konstantin (DESY)

Evidence for possible quantum spin-ice behaviour in Pr2Hf2o7 as seen by inelastic neutron scattering.

Content:

The 227 rare earth pyrochlore systems are well known for their diverse magnetic ground state due to quintenssential lattice for frustration and Ising anisotropy. A delicate competition of crystal field, exchange and dipolar interactions can lead to exotic magnetic ground state, such as spin-ice behaviour in Dy2Ti2O7 and Ho2Ti2O7 [1, 2]. The quantum spin-ice behavior is one of very interesting topic of current research from both experimental and theoretical perspectives. The light rare earth like Pr-based pyrochlores (Pr3+μeff= 3.58 μB) in which dipolar interaction is relatively weak seem to be potential candidate for such quantum fluctuation dominated physics. Furthermore, Pr3+ ion being a non-Kramers ion, introduces transverse terms in the effective spin-½ Hamiltonian of the system leading to a quantum spin-ice ground state [3].
Recently, the low temperature properties of Pr2Hf2O7 have been investigated by ac susceptibility and heat capacity which showed evidence for a slow spin-dynamics in this compound [4, 5]. The magnetic properties are well described by an effective spin-1/2 model with a very non-Ising contribution which is a favourable condition for the realization of quantum spin-ice behaviour. Inelastic neutron scattering (INS) show five dispersionless crystal field excitations due to crystal field effect. The INS data reveal the ground state to be doublet with significant mixing of |3H4, ±4 > with other multiplets [4, 5]. Such a mixing in ground state wave function can cause quantum fluctuations.
Motivated by the above interesting results, we extended the study using polarised and low energy neutron scattering on a Pr2Hf2O7 single crystal, grown by the floating zone technique. Polarised neutron diffraction measurements on D7 instrument, ILL in Grenoble, reveal the absence of any transition down to 85mK, diffuse scattering along the (H00) & (HHH) high symmetry directions and hints of pinch points. By comparing the results with the respective Q-map of Ho2Ti2O7 classical spin ice [6], the diffuse scattering is found along the same high symmetry directions, but is not as sharp, indicative of increased quantum fluctuations. Inelastic magnetic scattering measurements, performed at LET of ISIS, show energy dependent diffuse scattering along the same high symmetry directions. The inelastic data reveal absence of pinch points, which means that there is an increased amount of tetrahedra that violate the spin ice rule of 2 in 2 out. Low energy magnetic excitation bands (~ 0.3 meV) are present along the (H00) & (HHH) directions with a narrow band gap (~ 0.05meV). Although the data are yet to be fitted with theoretical models, comparison with literature shows that these features bear evidence of quantum spin ice behaviour. In the future an inelastic neutron scattering measurement of the single crystal Pr2Hf2O7, in an oriented external magnetic field, is planned in order to calculate the magnetic Hamiltonian of the system.

Primary authors:
Mr. SAMARTZIS, Alexandros (Helmholtz Zentrum Berlin)

Co-authors :
Prof. LAKE, Bella (Helmholtz Zentrum Berlin) Dr. ANAND, Vivek (Helmholtz Zentrum Berlin) Dr. ISLAM, Nazmul A.t.m (Helmholtz Zentrum Berlin) Dr. WILDES, Andrew (Institute Laue-Langevin) Dr. BEWLEY, Robert (Rutherford Appleton Laboratory)

Evolution of antiferromagnetic domains in the all-in-allout ordered pyrochlore Nd2Zr2O7

Content:

We report an observation of magnetic domains in the exotic, antiferromagnetically ordered all-in-all-out state of Nd2Zr2O7, induced by spin canting. Two different spin arrangements fulfill the Ising-like spin configuration. This leads to the occurrence of domains. While the two all-in-all-out spin arrangements occur equiprobable in zero field, the application of a magnetic field along the [111] direction allows for a manipulation of their domain structure. We have investigated Nd2Zr2O7 by means of static magnetization and dynamic susceptibility. The ground state is established in this compound below 0.31 K for external magnetic fields below 0.14 T. The magnetic domains are observed through a hysteresis of the susceptibility □ac(□). No hysteresis occurs, however, in the case of an external magnetic field □dc ‖ [100].

Primary authors:
Mr. OPHERDEN, Lars (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany)

Co-authors :
Mr. HORNUNG, Jacob (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Dr. HERRMANNSDöRFER, Thomas (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany) Mr. XU, Jianhui (Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany) Dr. ISLAM, A. T. M. Nazmul (Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany) Prof. LAKE, Bella (Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, 14109 Berlin, Germany) Prof. WOSNITZA, Joachim (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany)

Experimental realization of a quantum spin liquid in Ca10Cr7O28

Content:

Unlike conventional magnets where the magnetic moments are partially or completely static in the ground state, in a quantum spin liquid they remain in collective motion down to the lowest temperatures. Despite an extensive search among such compounds, experimental realizations remain very few. Here we investigate the new spin-1/2 magnet, Ca10Cr7O28, which has a unexplored lattice with several isotropic interactions consisting of strong ferromagnetic and weaker antiferromagnetic couplings. Bulk properties measurements, neutron scattering and muon spin relaxation reveal coherent spin dynamics in the ground state, the complete absence of static magnetism and diffuse spinon-like excitations. Thus we show experimentally that it displays all the features expected of a quantum spin liquid.

Primary authors:
Dr. BALZ, Christian (Helmholtz-Zentrum Berlin)

Co-authors :
Prof. LAKE, Bella (Helmholtz-Zentrum Berlin) Mr. SCHöNEMANN, Rico (Helmholtz-Zentrum Dresden-Rossendorf) Mr. OPHERDEN, Lars (Helmholtz-Zentrum Dresden-Rossendorf) Dr. HERRMANNSDöRFER, Thomas (Helmholtz-Zentrum Dresden-Rossendorf) Prof. REUTHER, Johannes (Helmholtz-Zentrum Berlin) Dr. RYLL, Hanjo (Helmholtz-Zentrum Berlin)

Exploring the Electronic Structure and Chemical Homogeneity of Individual Bi2Te3 Nanowires by Nano-Angle-Resolved Photoemission Spectroscopy

Content:

Due to their high surface-to-volume ratio, cylindrical Bi2Te3 nanowires are excellent model systems to investigate the chemistry and the unique conductive surface states of topological insulator nanomaterials. Here, we will present nano angle-resolved photoemission spectroscopy (nano-ARPES) measurements of individual cylindrical Bi2Te3 nanowires with a diameter of 100 nm. 1 The nanowires are synthesized by electrochemical deposition inside channels of ion-track etched polymer membranes.2 Core level spectra recorded with submicron resolution indicate a homogeneous chemical composition along individual nanowires, while nano-ARPES intensity maps reveal the valence band structure at the single nanowire level. First-principles electronic structure calculations for chosen crystallographic orientations are in good agreement with those revealed by nano-ARPES. The successful application of nano-ARPES on single one-dimensional nanostructures constitutes a new avenue to achieve a better understanding of the electronic structure of topological insulator nanomaterials.
1. J. Krieg, C. Chen, J. Avila, Z. Zhang, W. Sigle, H. Zhang, C. Trautmann, M.C. Asensio, M.E. Toimil-Molares, Nano Lett. 2016, 16, 4001.
2. O. Picht, S. Müller, I. Alber, M. Rauber, J. Lensch-Falk, D.L. Medlin, R. Neumann, M.E. Toimil-Molares, J. Phys. Chem. C 2012, 116, 5367.

Primary authors:
Dr. TOIMIL-MOLARES, Maria Eugenia (GSI Helmholtz Centre for Heavy Ion Research)

Co-authors :
Ms. KRIEG, Janina (GSI Helmholtz Centre for Heavy Ion Research) Ms. TRAUTMANN, Christina (GSI Helmholtz Centre for Heavy Ion Research)

Extreme-field physics in Penning traps

Content:

I will present the work being performed in the area of extreme-field physics using Penning traps at GSI and HIJ. This comprises three different Penning trap experiments which study highly charged ions under various aspects, mainly on the background of precision spectroscopy in the presence of the extreme fields of atomic nuclei, but also employing high-intensity and/or high-energy lasers. I thus briefly review the works of the ARTEMIS, SPECTRAP and HILITE collaborations.

Primary authors:
Dr. VOGEL, Manuel (GSI and HIJ)

Fabrication, Structure and Magnetic Behavior of Large Three-Dimensional Nanoparticle Supercrystals

Content:

Magnetic nanoparticle assemblies form a novel type of artificial material with promising combinations of properties that are rarely found in conventional systems. Due to their potential use in multifunctional materials, refrigeration, strong permanent magnets or spintronic devices, these materials have recently moved into the focus of intense research activities.
The understanding of the magnetic behavior of nanomaterials is challenging due to several size effects emerging at the nanoscale. In assemblies of nanoparticles these difficulties are even more pronounced because of inter-particle interactions and their complex interplay.
Hence, the fabrication of very large three-dimensional nanoparticle assemblies (nanoparticle macrocrystals) remains challenging.
We have succeeded in fabricating nanoparticle macrocrystals on length scales of 300-1000 µm by developing a novel centrifuge assisted sedimentation technique. Using 15 nm iron oxide nanoparticles which were characterized by SEM, magnetometry and scattering methods, nanoparticle macrocrystals were prepared with different process parameters. The resulting samples were investigated concerning their morphology, nanoparticle order and magnetic collective behavior. For this, various techniques like e.g. small angle scattering at the JCNS GALAXI were employed.

Primary authors:
Mr. SMIK, Michael (Forschungszentrum Jülich) Mrs. WILBS, Genevieve (Forschungszentrum Jülich)

Co-authors :
Dr. KENTZINGER, Emmanuel (Forschungszentrum Jülich) Mr. PERßON, Jörg (Forschungszentrum Jülich) Dr. RüCKER, Ulrich (Forschungszentrum Jülich) Dr. PETRACIC, Oleg (Forschungszentrum Jülich) Prof. BRüCKEL, Thomas (Forschungszentrum Jülich)

Fast synchrotron imaging of insects

Content:

In recent years, synchrotron-based X-ray microtomography became an established method for the 3D examination of insects. The imaging stations of KIT’s Institute for Photon Science and Synchrotron Radiation (IPS) are optimized for fast X-ray imaging, thus facilitating high throughput experiments and even in vivo studies on fast-moving animals. The talk features recent results of various fast X-ray imaging experiments on insects from different research fields, including functional morphology, paleontology and biomimetic design. Emphasis is also given to the (semi-) automated analysis of complex tomography data.

Primary authors:
Dr. VAN DE KAMP, Thomas (Karlsruhe Institute of Technology)

Co-authors :
Mr. DOS SANTOS ROLO, Tomy (Karlsruhe Institute of Technology) Dr. SCHWERMANN, Achim (Universität Bonn) Mr. LöSEL, Philipp (Universität Heidelberg) Prof. BAUMBACH, Tilo (Karlsruhe Institute of Technology)

First-order magnetization process as a tool of magnetic-anisotropy determination: the case of U3Cu4Ge4

Content:

Uranium-based intermetallic compounds often display very strong magnetic anisotropies, the energy of which is usually not directly accessible by common experimental methods. Here, we report on static- and pulsed-field studies of U3Cu4Ge4. This material orders ferromagnetically at TC = 73 K with the easy-magnetization direction along the a axis and a strong bc-plane anisotropy. The magnetization measured for fields along the hard b direction displays a first-order magnetization process that can be described well by use of a phenomenological theory yielding anisotropy constants up to the sixth order. This phenomenological description, working excellently for U3Cu4Ge4, may as well be applied for other uranium-based compounds.

Primary authors:
Dr. GORBUNOV, D.i. (Dresden High Magnetic Field Laboratory)

Co-authors :
Dr. HENRIQUES, M.s. (Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague, Czech Republic) Prof. ANDREEV, A.v. (Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague, Czech Republic) Dr. SKOURSKI, Y. (Dresden High Magnetic Field Laboratory) Dr. RICHTER, Manuel (IFW Dresden e.V., P.O. Box 270116, D-01171 Dresden, Germany) Dr. HAVELA, L. (Charles University in Prague, Faculty of Mathematics and Physics, Department of Condensed Matter Physics,Ke Karlovu 5, 121 16 Prague, Czech Republic) Prof. WOSNITZA, J. (Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum)

Flow-induced alignment of spindle shaped particles using microjets

Content:

Liquid jets are used at synchrotron and XFEL light sources allowing studies of structure and dynamics of soft condensed matter. We developed a liquid jet setup for x-ray scattering experiments on complex fluids that supports small and wide angle x-ray scattering geometries (SAXS and WAXS) [1]. The jet is formed by a gas dynamic virtual nozzle (GDVN) [2] producing diameters between 1 µm and 20 µm at a jet length of several hundred µm. The homogeneous and very thin liquid jets offer numerous advantages compared to conventional sample injection environments [1]. For instance, they allow measurements in a steady jet regime that breaks into a train of droplets cooling rapidly in vacuum and thus allowing studies on supercooled liquids [3].
In this presentation we will focus on two different studies using our liquids jet setup: 1. Flow-induced alignment of spindle shaped particles probed by WAXS.
2. Influence from refraction of X-rays from µm-sized jets and droplets on the SAXS patterns. These anisotropic patterns arise due to the cylindrical (jet) and spherical (droplets) geometries [4].
These results will be compared with similar data taken with different injection devices and the possibility of performing rheology studies at high shear rates using liquid jets will be discussed.

Primary authors:
Mrs. VALERIO, Joana (DESY)

Co-authors :
Dr. WALTHER, Michael (DESY) Dr. LEHMKUEHLER, Felix (DESY) Dr. JAIN, Avni (DESY) Dr. HOELTIG, Michael (DESY) Mrs. FRENZEL, Lara (DESY) Mr. VAKILI, Mohammad (Hamburg University) Dr. BOMMEL, Sebastian (DESY) Mrs. SHEYFER, Dina (DESY) Dr. SCHROER, Martin (EMBL) Prof. TREBBIN, Martin (Hamburg University) Dr. LAL, Jyotsana (Boston University) Dr. SPRUNG, Michael (DESY) Prof. GRUEBEL, Gerhard (DESY)

Grating-Based Phase-Contrast Computed Tomography at PETRA III

Content:

Phase-contrast imaging has proven to be a valuable tool when investigating weak absorbing material like soft tissue, due to its increased contrast compared to conventional absorption-contrast imaging.
Especially for investigating samples combined of weak and strong absorbing materials, grating-based phase-contrast (gbPCI) has an advantage against absorption-based contrast or propagation-based phase-contrast.
Main drawbacks of gbPCI are the time consumption due to the enlarged number of taken images and the limited resolution due to the influence of the gratings.
Here we will present our current instrumentation for both single-grating and double-grating interferometer which allows to minimise those limitations. Also we will show different examples of possible applications in the field of biomedical and materials science.

Primary authors:
Mr. HIPP, Alexander (Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. HERZEN, Julia (Technische Universität München) Dr. HAMMEL, Jörg (Helmholtz-Zentrum Geesthacht) Dr. BECKMANN, Felix (Helmholtz-Zentrum Geesthacht)

Ground state potential energy surfaces around selected atoms from resonant inelastic x-ray scattering

Content:

Thermally driven chemistry as well as materials' functionality are determined by the potential energy surface of a systems electronic ground state. This makes the potential energy surface a central and powerful concept in physics, chemistry and materials science. However, direct experimental access to the potential energy surface locally around atomic centers and to its long-range structure are lacking. Here we demonstrate how sub-natural linewidth resonant inelastic soft x-ray scattering (RIXS) at vibrational resolution is utilized to determine ground state potential energy surfaces locally and detect long-range changes of the potentials that are driven by local modifications. We show how the general concept is applicable not only to small isolated molecules such as O2 but also to strongly interacting systems such as the hydrogen bond network in liquid water. The weak perturbation to the potential energy surface through hydrogen bonding is observed as a trend towards softening of the ground state potential around the coordinating atom [1]. Furthermore, different RIXS channels in a molecule can act as selectitve gates to specific vibrational modes by means of core excited dynamics, allowing to probe directly the localized modes.
The instrumental developments in high resolution resonant inelastic soft x-ray scattering are currently accelerating and will enable broad application of the presented approach. With this multidimensional potential energy surfaces that characterize collective phenomena such as (bio)molecular function or high-temperature superconductivity will become accessible in near future.

[1] S. Schreck et al., Nature Scientific Reports 6 20054 (2016)

Primary authors:
PIETZSCH, Annette (Helmholtz-Zentrum Berlin)

Co-authors :
SCHRECK, Simon (Stockholm University) ECKERT, Sebastian (Universität Potsdam) JAY, Raphael (Universität Potsdam) NISKANEN, Johannes (HZB) FONDELL, Mattis (HZB) MIEDEMA, Piter S. (HZB) SåTHE, Conny (MAX IV Laboratory) TECHERT, Simone (DESY, MPI fuer Biophysikalische Chemie, Uni Göttingen) STROCOV, Vladimir N (PSI) SCHMITT, Thorsten (PSI) HENNIES, Fra´nz (MAX IV Laboratory) RUBENSSON, Jan-erik (Universität Uppsala) FöHLISCH, Alexander (HZB, Uni Potsdam)

HESAXS at HEMS

Content:

Recent improvements at the high energy material science beamline (HEMS) P07 at Petra 3 increased the accessible size resolution at high energy small angle x-ray scattering (HESAXS) experiments. A major part in reducing the background were the use of tungsten single crystals as slits. Additional changes in the detector setup increased the time resolution by a factor of six. Now, simultaneous XRD and SAXS measurements are possible with a time resolution of up to 1 second, dependent on the sample. We used a dilatometer to do in-situ measurements of carbide precipitation and growth in TiAl alloys as an example system to test the improved setup.
During the next run, a changed positioning of the slits and a new beamstop should further increase the space resolution.

Primary authors:
Mr. GAYER, Sören (Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. STARK, Andreas (Helmholtz-Zentrum Geesthacht) Dr. STARON, Peter (Helmholtz-Zentrum Geesthacht) Prof. PYCZAK, Florian (Helmholtz-Zentrum Geesthacht) Prof. SCHREYER, Andreas (ESS)

HILITE - A Penning trap to study interactions of ions with intense photon fields

Content:

We present a Penning trap setup for the preparation and storage of well-defined ion targets for studies of laser-ion-interaction at high laser field strengths. We explain the applied techniques for target preparation and non-destructive measurement of reaction products, and show the current status of the setup as well as data of characterizing measurements.

Primary authors:
Mr. RINGLEB, Stefan (Intitute of Optics and Quantumelectronics, Universität Jena) Mr. STALLKAMP, Nils (GSI Darmstadt)

Co-authors :
Dr. VOGEL, Manuel (Helmholtz-Institute Jena) Mr. KUMAR, Sugam (Inter-University Accelerator Centre New Delhi) Dr. QUINT, Wolfgang (Physikalisches Institut, Ruprecht Karls-Universität Heidelberg) Prof. STöHLKER, Thomas (Helmholtz-Insitute Jena) Prof. PAULUS, Gerhard G. (Intitute of Optics and Quantumelectronics, Universität Jena)

Hard X-ray Microscopy Station for Material Research at the Institute for Photon Science and Synchrotron Radiation, KIT

Content:

MiQA experimental station is a primary component of the project “Hard X-ray Microscopy for Material Research and Quality Assurance”. It was developed by the Institute for Photon Science and Synchrotron Radiation at Karlsruhe Institute of Technology. MiQA station is tailored for X-ray imaging at energies of up to 60 keV by means of 3D full-field and scanning microscopy, also combined with absorption and spectroscopic detectors. Grating interferometry and propagation based phase contrast imaging in both parallel and cone beam geometries are possible. Research and case studies include multiscale and multicontrast microscopy imaging of the internal structure of solar cells, batteries, catalysts, composite and alloy materials both in tomography and laminography modes, including in operando studies. Characterization of existing and emerging X-ray optical elements, such as gratings and x-ray lenses, is available at this station as well. The station is currently under acceptance tests. First trials with the X-ray beam are planned for the end of this year.

Primary authors:
Dr. SERGEY, Gasilov (Karlsruhe Institute of Technology)

Co-authors :
Dr. WEINHARDT, Venera (Karlsruhe Institute of Technology) Dr. HEINE, Ruth (Karlsruhe Institute of Technology) Prof. BAUMBACH, Gerd Tilo (Karlsruhe Institute of Technology)

Heterostructures of perovskite thin films

Content:

Due to electronic correlations and / or competing ordering phenomena, transition metal oxides (TMO) show functionalities which make them promising candidates for sensors or devices in future information technologies. Such devices will consist of heterostructures of different TMO's, where the interfaces play the crucial role. Due to the sensitivity of TMO's to external parameters such as strain, chemical and electronic doping, magnetic and electric fields etc., their properties are easily altered at the interface.
We will present results from two different perovskite heterostructures. First we studied the effect of temperature and magnetic fields on the interfacial magnetization of La{1/3}Sr{2/3}FeO{3} (LSFO) and La{2/3}Sr{1/3}MnO{3} (LSMO) heterostructures.LSFO and LSMO bulk systems have been well investigated in recent years, as they have very interesting properties. LSFO is a model system for a Verwey transition. For the used stoichiometry of LSFO, iron has the nominal valence of +3.67 composed of Fe^(3+) and Fe^(4+). At T{CO} = 200 K charge ordering sets in, where a charge disproportionation of Fe^(4+) into Fe^(3+) and Fe^(5+) occurs. This leads to a step-wise increase in resistivity, the so called Verwey transition. This “metal-insulator” transition is accompanied by a magnetic transition into an antiferromagnetic state. On the other hand LSMO is an oxide with a rich phase diagram and in the used stoichiometry LSMO is a ferromagnet with a T{C} = 335 K. The resistivity of LSFO increases by about 8 orders of magnitude between T{V} = T{CO} = T{N} = 200 K and 5 K, due to charge ordering and charge disproportionation. The electronic doping influences the interface behavior by potential changes of the charge carrier density at the interface and one expects a tuning of the hole density in LSMO.
The second system consists of a thin ferromagnetic La0.5Sr0.5MnO3 film grown on ferroelectric BaTiO{3}, combined as a heterostructure to create an artificial multiferroic material. We have chosen LSMO with a doping level of x=0.5 as it is close to a magnetic phase transition from a ferromagnetic to an antiferromagnetic phase. Burton et al. [1] claimed that it should be possible to drive the magnetic order to an antiferromagnetic structure by the application of electric fields. The polarization direction of the BTO leads to bound charges in the BTO which induces a screening effect in the LSMO by charge accumulation or depletion at the interface depending on the polarization direction. We intended to prove that experimentally by measuring the magnetization of the LSMO film on BTO with a SQUID during the application of an electric field.

Reference: [1] Burton et. al, PRB, 80 (2009)

Primary authors:
Dr. SCHRöDER, Sonja (Jülich Centre for Neutron Science JCNS , Forschungszentrum Jülich, Jülich, Germany)

Co-authors :
Dr. SCHMITZ, Markus (Jülich Centre for Neutron Science JCNS , Forschungszentrum Jülich, Jülich, Germany) Mr. WASCHK, Markus (Jülich Centre for Neutron Science JCNS , Forschungszentrum Jülich, Jülich, Germany) Dr. ZAKALEK, Paul (Jülich Centre for Neutron Science JCNS , Forschungszentrum Jülich, Jülich, Germany) Dr. VOIGT, Jörg (Jülich Centre for Neutron Science JCNS-FRM-II, Forschungszentrum Jülich, Jülich, Germany) Prof. BRüCKEL, Thomas (Jülich Centre for Neutron Science JCNS , Forschungszentrum Jülich, Jülich, Germany)

High efficiency gratings based on asymmetric-cut multilayers

Content:

We demonstrated a novel way to extend the size of highly dispersive gratings based on asymmetric-cut multilayers. Such gratings can be used as efficient monochromators, spectrometers or for pulse compression of FEL pulses.

Primary authors:
Dr. PRASCIOLU, Mauro (DESY)

Co-authors :
Dr. BAJT, Sasa (DESY)

High precision laser spectroscopy of highly charged ions: Resonant excitation of Li-like Kr33+ at 136 eV and perspectives for hyperfine structure studies at highest Z with FLASH

Content:

We report on high-resolution spectroscopy measurements of the 2 2S1/2 – 2 2P3/2 fine-structure transition of Li-like Kr33+ ions trapped in an electron beam ion trap (EBIT) and resonantly excited by soft X-ray photons at 136 eV produced by the Free Electron Laser in Hamburg FLASH. Generally, investigations of such transitions in highly charged Li-like ions are of great interest since they in principle enable precision tests of quantum electrodynamics (QED) at strong fields. A preliminary data analysis results in the measured transition energy of 136.189(6) eV with an accuracy of below 50 ppm, improving the so far best measurement value [1] by a factor of 6. The new value is in excellent agreement with recent theoretical calculations including relativistic recoil, electron-correlation and QED effects [2]. We will also discuss the perspectives for hyperfine structure studies in heavy Li-like systems like Bi80+ utilizing the EBIT and the high resolution PG monochromator beamline at the FLASH facility. Using the same measurement technique as for Li-like Krypton should allow us to reach an accuracy level needed to disentangle contributions from nuclear size effects and QED to the hyperfine splitting energy and by that enabling us for the first time to test QED-contributions in the regime of strong electromagnetic fields at highest Z on a few percent level.

Primary authors:
Dr. BRENNER, Günter (DESY Hamburg)

Co-authors :
BERNITT, Sven (Max-Planck-Institut für Kernphysik, Heidelberg) BLESSENOHL, Michael (Max-Planck-Institut für Kernphysik, Heidelberg) DOBRODEY, Stepan (Max-Planck-Institut für Kernphysik, Heidelberg) CIELUCH, Andre (Max-Planck-Institut für Kernphysik, Heidelberg) STEINBRüGGE, Rene (Max-Planck-Institut für Kernphysik, Heidelberg) EPP, Sascha (Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg) CRESPO LóPEZ-URRUTIA, José Ramon (Max-Planck-Institut für Kernphysik, Heidelberg)

High purity x-ray polarimetry with single-crystal diamonds

Content:

The detection of vacuum birefringence induced by a large electric field requires an extremely high polarization purity in the order of 10^-11 at a photon energy of 12keV. With present x-ray polarizers based on silicon channel-cut crystals using multiple consecutive crystal reflections a polarization purity of 2.4 ·10^-10 at a photon energy of 6.44 keV can be reached [1]. Special developed quasi channel-cut mounts enable the use different small single crystals such as diamond and quartz for high-purity x-ray polarimetry.
We report on the use of synthetic single-crystal diamonds for high purity x-ray polarimetry to improve the polarization purity of present-day x-ray polarimeters. The polarimeter setup consists of a polarizer and an analyzer, each based on two parallel diamond crystals used at scattering angles very close to 90°, i.e. a direct derivative of the scheme used by Barkla in 1903 to demonstrate the electromagnetic nature of x-rays. The experiment was performed using one (400) Bragg reflection on each diamond crystal and synchrotron undulator radiation at an x-ray energy of 9838.75 eV. A polarization purity of 8.9·10^-10 was measured at the European Synchrotron Radiation Facility, which is the best value reported for two-reflection polarizer/analyzer setups. This result is encouraging and is a first step to improve the resolution of x-ray polarimeters further by using diamond crystal polarizers and analyzers with four or six consecutive reflections.[2]

References
[1] B. Marx, K. S. Schulze, I. Uschmann, T. Kämpfer, R. Lötzsch, O. Wehrhan, W. Wagner, C. Detlefs, T. Roth, J. Härtwig, E. Förster, T. Stöhlker and G. G. Paulus, Phys. Rev. Lett. 110, 254801 (2013)
[2] H. Bernhardt, B. Marx-Glowna, K. S. Schulze, B. Grabiger, J. Haber, C. Detlefs, R. Loetzsch, T. Kämpfer, R. Röhlsberger, E. Förster, T. Stöhlker, I. Uschmann, G. G. Paulus, Appl. Phys. Lett. 109, 121106 (2016)

Primary authors:
Mr. BERNHARDT, Hendrik (Helmholtz Institute Jena)

Co-authors :
Mrs. MARX-GLOWNA, Berit (Institute for Optics and Quantum Electronics Jena) Dr. SCHULZE, Kai-sven (Helmholtz Institute Jena) Mr. GRABIGER, Benjamin (Helmholtz Institute Jena) Ms. SCHMITT, Annika (Institute for Optics and Quantum Electronics Jena) Mr. HABER, Johann (Deutsches Elektronen-Synchrotron DESY) Mr. DETLEFS, Carsten (European Synchrotron Radiation Facility) Dr. LöTZSCH, Robert (Helmholtz Institute Jena) Prof. RöHLSBERGER, Ralf (Deutsches Elektronen-Synchrotron DESY) Prof. FöRSTER, Eckhart (Helmholtz Institute Jena) Prof. STöHLKER, Thomas (Helmholtz Institute Jena) Dr. USCHMANN, Ingo (Helmholtz Institute Jena) Prof. PAULUS, Gerhard G. (Helmholtz Institute Jena)

High resolution x-ray focusing with multilayer Laue lenses

Content:

We present recent results in imaging at PETRA III P11 with two crossed high numerical aperture wedged multi-layer Laue lenses, producing a 2D focus. Rich in strontium, and carried across the globe from Antarctica, the Acantharia protozoa provides a beautiful test sample due to its high contrast and intricate skeletal structure. This sample was imaged with two lens sets, of numerical apertures 0.008 and 0.016, with a scattering efficiency of 65%.

Primary authors:
Dr. MORGAN, Andrew (CFEL, DESY)

Co-authors :
Dr. BAJT, Saša (DESY)

High-energy SAXS for the in situ study of precipitation kinetics in an Al-Mg-Zn alloy under friction stir welding thermal cycles

Content:

Various Al alloys for structural applications (e.g. AA2xxx or AA7xxx) are strengthened by nano-precipitates. The strengthening precipitates are strongly influenced by welding-induced thermal cycles that can reduce material performance under service conditions. Friction stir welding (FSW) is a joining technique used for the production of Al structures e.g. in aerospace and shipbuilding industries. Thus, the precipitation kinetics in an Al-2.1Mg-8.4Zn alloy (wt%) developed for aircraft construction was studied under thermal cycles as they occur in friction stir welding.
A commercial quenching and deformation dilatometer (TA Instruments 805A/D) was used at HZG beamline HEMS (P07) at PETRA III at DESY for simulating the welding thermal cycles in small samples. Small-angle X-ray scattering (SAXS) at a photon energy of 70 keV was used to monitor volume fraction and mean size of nano-precipitates during thermal cycles. High X-ray energies allow using thick samples that can be further processed afterwards. With the dilatometer, the thermal influence of the friction stir welding process can easily be studied in-situ, varying the maximum temperature and cycle time.
In addition, a numerical model was implemented for predicting the precipitation kinetics in the ternary Al-Mg-Zn alloy during thermal welding cycles. The model calculates the development of precipitate size distributions of the metastable eta’ phase and the stable eta phase during all stages of precipitation, i.e. nucleation, growth, and coarsening. After calibrating the model parameters with the results of SAXS measurements, predictions in a wider range of temperatures and cycle times and for different tempers of the starting material are possible.

Primary authors:
Dr. STARON, Peter (Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. FISCHER, Torben (Helmholtz-Zentrum Geesthacht) Dr. STARK, Andreas (Helmholtz-Zentrum Geesthacht)

Higher-order correlations and the glass transition of complex liquids

Content:

Although glasses are very common in everyday life, the glass transition is one of the mysteries in condensed matter physics. Upon approaching this transition, the sample dynamics slows down by orders of magnitude while the static structure remains almost unchanged. In addition, relaxation phenomena become non-exponential pointing to a broad distribution of relaxation times and the existence of dynamical heterogeneities, suggested to be closely connected to spatial heterogeneities. Simulations and theory show that the study to higher-order structure and dynamics will help to uncover the glass transition phenomenon, however, experimental access to higher-order structure is challenging. Here, we will discuss the potentials of higher-order correlation functions from coherent X-ray scattering experiments on colloidal samples in order to obtain structure and dynamics in the vicinity of their glass transition.
First, we will present a microrheology study on the dynamics of polypropylene-glycol by means of X-ray photon correlation spectroscopy (XPCS) approaching the glass transition temperature Tg [1]. Beside a cross-over from Brownian motion to hyperdiffusive and ballistic dynamics, dynamical heterogeneities increase dramatically upon cooling. This leads to two effects: a) increasing spatial heterogeneity and b) correlated motion at temperatures close to and below 1.12 Tg. Second, we will discuss structural higher-order correlations in colloidal systems by means of X-ray cross correlation analysis (XCCA) [2]. Examples of structure formation in thin colloidal films and colloidal crystals will be presented [3-5]. Special attention is paid to hard spheres systems. Beside correlations in hard-sphere crystals [4], we studied structure formation and dynamics in densely-packed liquid and glassy states. With increasing volume fraction, we observe a growth of medium-range order in colloidal glasses and appearance of ordered clusters prior to the glass transition and crystallisation. Both observations are characterized by a connection of increasing structural higher-order correlations and slowing down of the sample – providing new insights to the glass transition of colloidal systems.
[1] H. Conrad, F. Lehmkühler, B. Fischer et al. Phys. Rev. E 91, 042309 (2015).
[2] F. Lehmkühler, G. Grübel and C. Gutt. J. Appl. Cryst. 47, 1315 (2014).
[3] M.A. Schroer, F. Westermeier, F. Lehmkühler et al. J. Chem. Phys. 144, 084903 (2016).
[4] F. Lehmkühler, B. Fischer, L. Müller, B. Ruta and G. Grübel. in review (2016).
[5] M.A. Schroer, C. Gutt, F. Lehmkühler et al. Soft Matter 11, 5465 (2015).

Primary authors:
Dr. LEHMKüHLER, Felix (DESY)

Co-authors :
Dr. SCHROER, Martin (EMBL) Prof. GRüBEL, Gerhard (DESY)

Highly ordered 3D nanoparticle superlattices investigated by microresonator ferromagnetic resonance

Content:

Magnetic nanoparticles and their assembly into highly correlated superstructures are of great interest for future applications, e.g. as material for magnon-spintronic. These systems are not only distinguished by the obvious miniaturization but by their novel physical properties emerging due to their limited size and ordered arrangement. These superstructures are formed from nanometer-sized building blocks ordered like atoms in a crystal, which render them a new class of materials.
Recently, single micrometer-sized three-dimensional magnetic nanoparticle assemblies (so-called mesocrystal) became available, exhibiting a high degree of structural order close to that of an atomic crystal. These systems provide a good basis for the magnetic investigation of nanoparticle superstructures.

Novel Microresonators, provide the necessary sensitivity for the investigation of static and dynamic magnetic properties of nano- and micrometer-sized objects using ferromagnetic resonance (FMR) [1,2]. Due to the much higher filling factor as compared to conventional microwave cavities, they offer several orders of magnitude increased sensitivity gain. A focused ion beam (FIB)[3] was used to isolate an individual 3D mesocrystal from an ensemble [4] and to transfer it into the microresonator loop (see Fig. 1). The FMR study reveals the magnetic anisotropy of the single mesocrystal, which is corroborated by micromagnetic simulations. It was possible for us to functionalize the system and to switch between two anisotropy components.

[1] A. Banholzer, R. Narkowicz, C. Hassel, R. Meckenstock, S. Stienen, O. Posth, D. Suter, M. Farle, and J. Lindner, Nanotechnology 22, 295713 (2011)
[2] C. Schoeppner, K. Wagner, S. Stienen, R. Meckenstock, M. Farle, R. Narkowicz, D. Suter, and J. Lindner, J. Appl. Phys. 116, 033913 (2014)
[3] D. Meertens, M. Kruth, and K. Tillmann, Journal of large-scale research facilities 2, (2016)
[4] S. Disch, E. Wetterskog, R.P. Hermann, G. Salazar-Alvarez, P. Busch, T. Brückel, L. Bergström and S. Kamali, Nano Lett., 10, 799 (2010)

Primary authors:
Dr. JOSTEN, Elisabeth (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Dr. NARKOWICZ, Ryszard (HZDR) Dr. KáKAY, Attila (HZDR) MEERTENS, Doris (FZJ-ERC) Prof. BERGSTRöM, Lennart (Stockholm University) Dr. LENZ, Kilian (HZDR) Dr. LINDNER, Jürgen (HZDR) Prof. FASSBENDER, Jürgen (HZDR) Prof. BRüCKEL, Thomas (FZJ)

Imaging molecular electron dynamics with time- and angle-resolved photoelectron spectroscopy

Content:

We theoretically study how time- and angle-resolved photoemission spectroscopy can be applied for imaging coherent electron dynamics in molecules [1]. We consider a process in which a pump pulse triggers coherent electronic dynamics in a molecule by creating a valence electron hole. An ultrashort extreme ultraviolet probe pulse creates a second electron hole in the molecule. Information about the electron dynamics is accessed by analyzing angular distributions of photoemission probabilities at a fixed photoelectron energy. We demonstrate that a rigorous theoretical analysis taking into account the indistinguishability of transitions induced by the ultrashort, broadband probe pulse and electron hole correlation effects, is necessary for the interpretation of time- and angle-resolved photoelectron spectra. We show how a Fourier analysis of time- and angle-resolved photoelectron spectra from a molecule can be applied to follow its electron dynamics by considering photoelectron spectra from an indole molecular cation with coherent electron dynamics.
[1] Daria Popova-Gorelova, Jochen Küpper and Robin Santra, Phys. Rev. A 94, 013412 (2016).

Primary authors:
Dr. GORELOVA, Daria (CFEL, DESY)

In situ GISAXS analysis of spray deposited biopolymer/ inorganic nanoparticle composites

Content:

Metal-biopolymer nanocomposites based on cellulose nanocrystals (CNCs) are gaining wide interest for nanotechnology such as organic electronics, solar cells or diagnostics. In combination with plasmonic silver nanoparticles (Ag NPs), arranged as multilayer structures, these composite materials can be used as sensors for surface enhanced Raman spectroscopy (SERS), antibacterial packaging material or conductive and flexible substrates. For effective industrial fabrication not only the controlled arrangement of the CNCs and Ag NPs during the deposition process is essential but also the use of an industrial compatible deposition process. Air-brush spray deposition is a versatile deposition technique that fulfills industrial demands and was thus chosen for preparation of cellulose/ Ag NP composites.

We investigated all spray deposited cellulose/ Ag NP multilayer and the single cellulose and Ag NP layer respectively. By employing short spray pulses with drying time in-between compact cellulose thin films with tunable thicknesses were achieved. GISAXS measurements in combination with AFM revealed the inner structure of these cellulose layers that consist of agglomerated cellulose nanofibrils with broad distribution of the lateral length scales. Spray deposition of Ag NP on Si substrates resulted in large NP agglomerates identified in SEM as well as AFM measurements. The corresponding GISAXS pattern showed, additional to the high q structure signal associated to the NP diameter, a low q signal. This structure size can be assigned to NP agglomerates. For Ag NP deposited on cellulose thin films the low q structure signal resulting from Ag NP agglomerates could not be identified indicating that the Ag NP agglomeration is reduced when the nanoparticles are deposited on cellulose thin films. This result could be confirmed by SEM images.

Primary authors:
Dr. OHM, Wiebke (Desy Hamburg)

Co-authors :
Dr. BEYERSDORFF, Björn (Desy Hamburg) Mr. GENSCH, Marc (Desy Hamburg) Mr. MöLLER, Marcel (Desy Hamburg) Dr. PLECH, Anton (Karlsruhe Institute of Technology) Dr. STANIEC, Paul (Diamond Light Source) Dr. YU, Shun (KTH) Dr. KöRSTGENS, Volker (Technische Universität München) Prof. MüLLER-BUSCHBAUM, Peter (Technische Universität München) Prof. ROTH, Stephan (Desy Hamburg)

In situ GISAXS investigation of Al growth on a diblock copolymer substrate

Content:

Aluminum is sputter deposited on a nanostructured PS-b-PMMA substrate where it forms self assembeled metal nanostructures that immitate the structure of the polymer substrate. To better understand the growth behaviour on the diblock in situ GISAXS investigation of Al deposition on the constituent homopolymers of the diblock (PS and PMMA) were also carried out.

Primary authors:
Dr. BEYERSDORFF, Björn (DESY)

Co-authors :
Dr. SCHWARTZKOPF, Matthias (DESY) Dr. OHM, Wiebke (DESY) Mr. HINZ, Alexander (Christian-Albrechts-Universität zu Kiel) Dr. THOMAS, Strunskus (Christian-Albrechts-Universität zu Kiel) Dr. POLONSKYI, Oleksandr (Christian-Albrechts-Universität zu Kiel) Prof. FAUPEL, Franz (Christian-Albrechts-Universität zu Kiel) Dr. KöRSTGENS, Volker (Technische Universität München) Ms. LöHRER, Franziska (Technische Universität München) Prof. MüLLER-BUSCHBAUM, Peter (Technische Universität München) Prof. ROTH, Stephan V. (DESY)

In situ materials characterisation with SRµCT

Content:

X-ray computed tomography is an ideal non-destructive tool for studying the inner structure of materials in three dimensions quantitatively. The Imaging Beamline P05 (IBL) operated by HZG at the PETRA III storage ring (German Electron Synchrotron - DESY, Hamburg) is dedicated to material sciences, offering a micro- and nano-tomography end station with high density and spatial resolution.
The high flux and coherence at the PETRA III storage ring opens up unique possibilities in the field of imaging techniques. Together with the extended space provided at the PO5 beamline for interchangeable sample environments this allows for time resolved in-situ measurements and applications at high density and spatial resolution. In the context of the available energy range from 5 to 50 keV this beamline is ideally suited for a broad range of applications in the field of materials science, biomaterials and bio inspired material engineering.
Here, we present an overview of the available experimental setup and imaging modes followed by exemplary results obtained at the micro tomography station from users and in house research in the field of materials, medical, biological, geological, and engineering sciences at different energies and spatial resolutions.

Primary authors:
Dr. HAMMEL, Jörg (Helmholtz-Zentrum-Geesthacht)

Co-authors :
Dr. GREVING, Imke (Helmholtz-Zentrum-Geesthacht) Dr. LOTTERMOSER, Lars (Helmholtz-Zentrum-Geesthacht) HIPP, Alexander (Helmholtz-Zentrum-Geesthacht) DOSE, Thomas (Helmholtz-Zentrum-Geesthacht) BURMESTER, Hilmar (Helmholtz-Zentrum-Geesthacht) WILDE, Fabian (Helmholtz-Zentrum-Geesthacht) ZELLER-PLUMHOFF, Berit (Helmholtz-Zentrum-Geesthacht) MOOSMAN, Julian (Berit.Zeller-Plumhoff@hzg.de) BECKMANN, Felix (Berit.Zeller-Plumhoff@hzg.de)

In-situ Scattering Experiments on the Structural and Morphological Changes of Metal Phosphides as Anode Materials in Lithium-Ion Batteries

Content:

The binary metal phosphides (M-P, M= Cu, Fe, Sn, Sb) compounds are of great interest as negative electrode materials for high energy density lithium-ion batteries. However, the morphology and structural changes at the nanoscale upon electrochemical (de)lithiation are not clear yet, which require further detailed investigation. In-situ neutron scattering technique was utilized to investigate and compare the morphological changes of copper phosphide and tin phosphide during the initial cycle. By coupling with SEM investigation, the surface activities of the electrodes at different electrochemical state, including the SEI formation, swelling and recovering, cracks appearance and stripping at nanoscale of the material particles are evaluated. With in-situ XRD measurement, the energy storage mechanism was further explained. This work demonstrates useful techniques to analyze the detailed fatigue mechanisms of the active material, and provides new insights of the nanostructural changes of anode materials reacting with lithium via conversion and alloying.

Primary authors:
Dr. FRIELINGHAUS, Henrich (Forschungszentrum Jülich GmbH, JCNS at MLZ)

Co-authors :
Dr. HE, Xin (Forschungszentrum Jülich GmbH, Helmholtz Institute Münster) WANG, Rui (Forschungszentrum Jülich GmbH, JCNS at MLZ) Dr. STAN, Marian Christian (University Münster, MEET Battery Research Center) Dr. PAILLARD, Elie (Forschungszentrum Jülich GmbH, Helmholtz Institute Münster) Dr. WANG, Jun (University Münster, MEET Battery Research Center) Dr. LI, Jie (University Münster, MEET Battery Research Center)

In-situ XAS on Li-Ion batteries during electrochemical cycling

Content:

Due to the nanocrystalline structure of the Li-Ion batteries in-situ-XAS is well suited to give in combination with x-ray diffraction and Li MAS NMR detailed information about structural changes during electrochemical cycling. The presentation will focus on the ultra-fast and reliable XAS data evaluation and the results of the principle component analysis to probe the reversibility of structural changes.

Primary authors:
Dr. MANGOLD, Stefan (Karlsruher Institut für Technologie)

Co-authors :
Dr. INDRIS, Silvio (KIT-)

In-situ studies of pure metal nanoparticle synthesis by laser ablation

Content:

Pulsed laser ablation synthesis in liquids [1] is a procedure to fabricate suspended nanoparticles from very different kind of solids. It is particularly useful for applications, where pure nanoparticles without stabilizers or reaction side products are required. These particles can be hybridized with e.g. biomolecules for biomedical applications or used in printable or self-assembled electronics [2]. The processes within the ablation dynamics are multiscale and involve plasma formation, atom condensation, primary particle formation and all kind of secondary agglomeration processes on a (sub)microsecond time scale. Understanding these reactions is particularly difficult, as they involve nanoscale structure formation, fast reactions and hindered access within the cavitation bubble inside the liquid. Within this project several hierarchical aspects of this process are addressed in order to gain a more complete picture of the dynamics as well as the factors that determine the definition and yield of the desired nanoparticles. The approach involves the application of stroboscopic small-angle X-ray scattering [3,4], ultrafast imaging with X-rays [5] and visible light [6,7] as well as spectroscopy [8]. For the first time it was possible to identify the nanoparticular matter with microsecond time resolution and its interaction with ligands [9] and with macroscopic structure formation of the laser-induced cavitation.

We would like to acknowledge beamtime at SLS, ESRF and ANKA and help by A. Diaz, T. Müller, A. Rack and D. Issenmann. This work is supported within priority program 1327 and the Heisenberg fellowship of the DFG. Discussions with S. V. Roth and W. Ohm on the applications in organic electronics are acknowledged.

[1] Amendola, V.; Meneghetti , M.; Phys. Chem. Chem. Phys. 2013,15, 3027.
[2] Roth, S. V. J. Phys.: Cond. Mat. 2016, 28, 403003.
[3] Wagener, P.; Ibrahimkutty, S.; Menzel, A.; Plech, A.; Barcikowski, S. Phys. Chem. Chem. Phys. 2013, 5, 3068.
[4] Ibrahimkutty, S.; Wagener, P.; Menzel, A.; Plech, A.; Barcikowski, S. Appl. Phys. Lett. 2012, 101, 103104.
[5] Ibrahimkutty S.; Wagener, P.; dos Santos Rolo, T.; Karpov, D.; Menzel, A.; Baumbach, T.; Barcikowski, S.; A. Plech, A. Sci. Rep. 2015, 5, 16313.
[6] Reich, S.; Schönfeld, P.; Wagener, P.; Letzel, A.; Gökce, B.; Menzel, A.; dos Santos Rolo, T.; Barcikowski, S.; Plech, A. J. Coll. Interf. Sci. 2016 accepted.
[7] Kohsakowski , S.; Gökce, B.; Tanabe, R.; Wagener, P.; Plech, A.; Ito, Y.; Barcikowski, S. Phys. Chem. Chem. Phys. 2016, 18, 16585.
[8] Reich, S.; Schönfeld, P.; Letzel, A.; Kohsakowski, S.; Gökce, B.; Barcikowski, S.; Olbinado, M.; Plech, A. ChemPhysChem 2016, submitted.
[9] Letzel, A.; Gökce, B.; Wagener, P.; Ibrahimkutty, S.; Menzel, A.; Plech, A.; Barcikowski, S. 2016 submitted.

Primary authors:
Dr. PLECH, Anton (Karlsruhe Institute of Technology)

Co-authors :
Mr. REICH, Stefan (Karlsruhe Institute of Technology) Mr. SCHöNFELD, Patrick (Karlsruhe Institute of Technology) Mr. DOS SANTOS ROLO, Tomy (Karlsruhe Institute of Technology) Prof. BAUMBACH, Tilo (Karlsruhe Institute of Technology) Mr. LETZEL, Alexander (Technical Chemistry, U. Essen-Duisburg) Mr. KOHSAKOWSKI, Sebastian (Technical Chemistry, U. Essen-Duisburg) Dr. GöKCE, Bilal (Technical Chemistry, U. Essen-Duisburg) Dr. WAGENER, Philip (Technical Chemistry, U. Essen-Duisburg) Prof. BARCIKOWSKI, Stephan (Technical Chemistry, U. Essen-Duisburg) Dr. IBRAHIMKUTTY, Shyjumon (MPI for Solid State Research, Stuttgart) Dr. MENZEL, Andreas (PSI Villigen) Dr. OLBINADO, Margie (ESRF, Grenoble)

In-situ tensile texture study of a new high plasticity Mg-RE alloy

Content:

A new Mg-RE (rare earth) alloy was previously developed by micro-alloying method (RE< 0.4 wt.%), which achieves a high ductility and good corrosion resistance. In-situ tensile test via neutron diffraction were performed to investigate first the deformation behaviour; and second the texture evolution which can be related to the deformation mechanism, and finally to understand why the as-cast Mg-RE alloys show such a high tensile ductility. Preliminary results showed that a dominated basal fibre texture was gradually developed with the increase of tensile strain. However, before the sample was broken a (10.0) fibre texture showed a similar intensity to that in (00.2), which means more activations of the non-basal slip planes during tensile deformation. This could also contribute to a relatively high elongation of this new Mg-RE alloy at room temperature. Further discussion will be showed together with the microstructures.

Primary authors:
Dr. GAN, Weimin (GEMS at MLZ, Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. HUANG, Yuanding (Magnesium Innovation Centre, Helmholtz-Centre Geesthacht) Dr. HOFMANN, Michael (Technische Universität München) Prof. KAINER, K.u. (Magnesium Innovation Centre, Helmholtz-Centre Geesthacht) Dr. HORT, N. (Magnesium Innovation Centre, Helmholtz-Centre Geesthacht)

In-situ time-resolved XRD and RHEED study of the polytypism in GaAs nanowires

Content:

The integration of III-V semiconductors on silicon is of particular interest to combine the standard semiconductor platform with direct band-gap materials, e.g. for on-chip optical communications. One approach to overcome the lattice mismatch between both material systems is the growth of III-V nanowires onto silicon substrates.
With a portable MBE system for in-situ X-ray investigations [1], we have studied the Zincblende (ZB) – Wurtzite (WZ) polytypism in gallium arsenide nanowires [2,3]. The current setup allows for simultaneous time-resolved investigation of crystal structure evolution by means of X-ray diffraction (XRD) and by Reflecting High-Energy Electron Diffraction (RHEED) during the complete growth process.
The combination of these complementary methods provides detailed information on crystal structure and the distribution of WZ and ZB segments within the nanostructures. While XRD gives access to the shape and the crystal structure of the whole illuminated NW ensemble under inspection, RHEED as a surface sensitive technique offers the possibility to analyse the evolution of phases along the NW axis during the growth process.
In this contribution we demonstrate the feasibility of the approach at the example of the formation of crystal phases during self-catalysed growth of GaAs nanowires onto Si(111). By analysing the relative intensity of the RHEED diffraction spots as a function of growth time it is found that in case of gallium pre-deposition the probability of forming WZ is higher compared to ZB phase in the early stages of growth. In contrast, NWs grown without pre-deposition quickly tend to a low fraction of the WZ phase. The results are verified by comparison with the XRD data.

We would like to acknowledge Hans Gräfe, Bärbel Krause and Svetoslav Stankov at the UHV laboratory of the Institute of Photon Science and Synchrotron Radiation, KIT and Jörg Strempfer, Sonia Francoual and David Reuther at P09, PETRA III, Desy. The work was supported by the BMBF projects (05ES7CK) and (05K13PS3).

Primary authors:
Mr. JAKOB, Julian (Laboratory for Application of Synchrotron Radiation, Karlsruhe Institute of Technology)

Indium Sulfide Buffer Layers for Cu(In,Ga)(S,Se)2 Thin-Film Solar Cells - A Study Using Soft X-Ray and Electron Spectroscopy

Content:

Thin-film solar cells based on Cu(In,Ga)(S,Se)2 (CIGSSe) absorbers achieve efficiencies greater than 22%. Typically, a chemical-bath-deposited CdS buffer is used for highest efficiencies. In order to integrate the buffer layer deposition into a dry in-line production process, promising alternatives (e.g., indium sulfide (InxSy) and zinc-oxy-sulfide) are currently being developed. An important prerequisite for improving the efficiency of cells based on these “new” heterojunctions is a detailed knowledge of the chemical and electronic structure of the buffer/absorber interface.
In this study, we use a unique combination of soft x-ray and electron spectroscopies, namely x-ray emission spectroscopy (XES) and x-ray photoelectron spectroscopy (XPS) to study the chemical and electronic structure of the InxSy/CIGSSe interface, thus providing crucial input for further improvement of the device structure. As grown, no diffusion of absorber elements into the InxSy buffer layer is observed. Upon thermal treatments that simulate subsequent cell processing steps, a distinct diffusion of copper and sodium from the absorber into the buffer layer is observed. This diffusion extends throughout the layer, indicating the formation of a copper−indium−sulfide phase. Furthermore, a correlation with reflection electron energy loss spectroscopy (REELS) is used to gather fundamental information about the optical properties of the InxSy and CIGSSe surfaces, e.g., a reduction of the InxSy surface band gap upon the thermal treatments.

Primary authors:
Dr. HAUSCHILD, Dirk (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT))

Co-authors :
Dr. MEYER, Frank (Exp. Physics VII, University of Wuerzburg) Mr. BENKERT, Andreas (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Dr. KREIKEMEYER-LORENZO, Dagmar (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Mrs. HANDICK, Evelyn (Exp. Physics VII, University of Wuerzburg) Prof. REINERT, Friedrich (Exp. Physics VII, University of Wuerzburg) Prof. HESKE, Clemens (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Dr. WEINHARDT, Lothar (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT))

Inelastic neutron scattering on the magnetocaloric compound MnFe4Si3

Content:

One way for saving energy in daily life is using the magnetocaloric effect (MCE), i.e. the change of magnetic entropy and adiabatic temperature following a change in an applied magnetic field. The ferromagnetic compound MnFe4Si3 (S.G.: P-6) is a promising candidate for applications. It has a magnetic phase transition in the range of 300 K and shows a moderate MCE of 2.9 J/kg/K at a reasonable magnetic field change from 0 T to 2 T. In order to understand the fundamental driving forces of the MCE in this material a study of magnetism, lattice dynamics and their interaction is necessary. X-ray as well as polarized and unpolarized inelastic neutron scattering at energies mainly below 20 meV have been performed looking for lattice (acoustic phonons) and magnetic excitations. Preliminary results at 1.5K indicate stronger magnetic interactions in [001] than [100] direction of the hexagonal system. The up to now measured excitations indicate that the magnon branch near the zone boundary along [h00] falls exactly on the transverse phonon branch propagating along [h00] and polarized in [00l], a remarkable fact evidenced by the combination of IXS and polarized INS used in this work. Measurements with polarized neutrons above TC reveal sizable magnetic fluctuations in a significant large temperature range (300...500K). Magnetic fluctuations in the paramagnetic phase are found to be isotropic. Simulations of spin waves in order to calculate values of the exchange interactions are ongoing.
Time of flight (TOF) measurements were performed at 4Seasons at JPARC at 7.5K and 360K. The collected data give us further insight in the excitation spectrum and provide more details for the map of the paramagnetic scattering above TC.

Primary authors:
Mr. BINISKOS, Nikolaos (Jülich Centre for Neutron Science (JCNS) at Institut Laue-Langevin (ILL), Forschungszentrum Jülich GmbH, Grenoble, France; CEA-Grenoble, INAC MEM MDN, Grenoble, France)

Co-authors :
Dr. SCHMALZL, Karin (Jülich Centre for Neutron Science (JCNS) at Institut Laue-Langevin (ILL), Forschungszentrum Jülich GmbH, Grenoble, France) Dr. RAYMOND, Stéphane (CEA-Grenoble, INAC MEM MDN, Grenoble, France) Dr. NEMKOVSKI, Kirill (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany) Dr. VOIGT, Jörg (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany; Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany) Mr. HERING, Paul (Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany) Mr. PERßON, Jörg (Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany) Dr. BOURDAROT, Frederic (CEA-Grenoble, INAC MEM MDN, Grenoble, France) Dr. BOSSAK, Alexei (European Synchrotron Radiation Facility, F-38043, Grenoble, France) Dr. SOULIOU, Sofia-michaela (European Synchrotron Radiation Facility, F-38043, Grenoble, France) Dr. KAJIMOTO, Ryoichi (Materials and Life Science Division, J-PARC Center, Japan Atomic Energy Agency, Tokai, Ibaraki, 319-1195, Japan) Dr. IIDA, Kazuki (Research Center for Neutron Science and Technology, Comprehensive Research Organization for Science and Society, Tokai, Ibaraki 319-1106, Japan) Prof. BRüCKEL, Thomas (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Garching, Germany; Jülich Centre for Neutron Science (JCNS) und Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany)

Influence of the coherence of FEL radiation on the multiphoton ionization of highly correlated quantum systems

Content:

Due to its superconducting accelerator technology FLASH at DESY can now deliver MHz pulse trains of 800 µs duration. By switching the electron bunch train generated by two injector lasers between FLASH1 and FLASH2 which equipped with two independent undulator beamlines, this allows to deliver the photon beam to two user experiments in parallel with individual selected photon beam parameters [1]. The unique features of FLASH2 such as utilization of the variable-gap undulator and improved electron beam diagnostics enable to vary photon properties as the wavelength and the pulse length but also the degree of transverse and longitudinal coherence of the FEL radiation independently from FLASH1. Recently, it was shown that at the FLASH2 the degree of coherence could be tuned within ~40-80% and confirmed by measuring the statistical pulse-to-pulse photon beam intensity distribution and applying an appropriate theoretical model [2, 3]. The latter may significantly extend the study of interaction of x-rays with matter in the non-linear regime of multiphoton processes. In this context, we propose to continue our investigations of multiphoton multiple ionization of Xe in the vicinity of the so-called 4d giant resonance in the extreme ultraviolet (EUV) range around 13 nm where extremely high charge states up to Xe^21+ were observed at irradiance levels of up to 10^16 W cm^-2 [4-6]. In fact, the role of giant reso¬nance and the impact of collective electron excitation by the intense radiation field on this exceptional behavior is controversially discussed with respect to the description of atomic multiphoton ionization in terms of collective plasma oscillations [7, and references therein]. The aim of our proposal is to study experimentally the dependence of multiphoton multi-ionization of Xe by ion yield spectroscopy in the giant resonance and non-resonance regime in the EUV range on the degree of longitudinal and transverse coherence taking exploiting the new excellent features of FLASH2. These investigations will help to clarify the situation because the different multiphoton ionization schemes (sequential, simultaneous, collective multiphoton excitation) should depend in different ways on different degrees of coherence of the FEL beam and hence a different coherence time. The proposed experiment is planned to be performed at the beamline FL24 at FLASH2 with a focused photon beam at irradiance ranging from 10^12 to 10^16 W cm^-2. The beam focusing will be realized by means of a KB bending mirror system which will be installed at the beamline in early 2017. Emphasis is laid on the quantitative determination of the beam parameters such as the photon pulse energy, the focused beam diameter, the pulse duration and the degree of FEL beam coherence in order to appropriately normalise and compare the different data sets for the scientific discussion. Moreover, our investigations will help to further characterize technical parameters of the beamline and to improve generally diagnostics methods at the FLASH2.

[1] B Faatz et al., New J. Phys. 18 (2016) 062002, Simultaneous operation of two soft x-ray free-electron lasers driven by one linear accelerator.
[2] E.A. Schneidmiller and M.V. Yurkov, J. Mod. Opt. 63, 293 (2016), Coherence properties of the radiation from FLASH.
[3] E.A. Schneidmiller and M.V. Yurkov, MOPOW013, Proceedings of IPAC2016, Busan, Korea, Application of statistical methods for measurements of the coherence of the radiation from SASE FEL.
[4] A.A. Sorokin et al., Phys. Rev. Lett. 99, 213002 (2007), Photoelectric effect at ultrahigh intensities.
[5] M. Richter et al., Phys. Rev. Lett. 102, 163002 (2009), Extreme ultraviolet laser excites atomic giant resonance.
[6] N. Gerken et al., Phys. Rev. Lett. 112, 213002 (2014), Time-Dependent Multiphoton Ionization of Xenon in the Soft-X-Ray Regime.
[7] M. Richter, J. Phys. B: At. Mol. Opt. Phys. 44, 075601 (2011), Atomic plasma excitations in the field of a soft x-ray laser.

Primary authors:
Dr. TIEDTKE, Kai (DESY Hamburg) Dr. SOROKIN, Andrey (DESY Hamburg) Dr. SHNEYDMILLER, Evgeny (DESY Hamburg)

Co-authors :
Dr. BRAUNE, Markus (DESY Hamburg) Dr. KLUMPP, Stephan (DESY Hamburg) Dr. KEITEL, Barbara (DESY Hamburg) Dr. YURKOV, Mikhail (DESY Hamburg) Dr. MEYER, Michael (XFEL) Ms. MERTENS, Karolin (UNI Hamburg) Dr. MARTINS, Michael (UNI Hamburg) Prof. RICHTER, Mathias (PTB Berlin)

Inner shell excitation of Mn with short intense x-ray pulses

Content:

Within one single pulse of a FEL like FLASH at DESY in Hamburg, with a duration in the order of 10fs the neutral xenon atom can absorb more than 50 photons and hence can be ionised up to Xe(21+). The physics driving the ionisation to this high charge state is still under debate, but it is presumed that the existence of resonances of the neutral atom and the intermediate (highly charged) ions play an important role in the sequential absorption process of so many photons.
By varying the atomic target from Xe, with its completely filled 4d subshell, to Mn, with its half filled 3d subshell, we study the influence of the correlative nature of the resonances involved in the photoionisation process.
The atomic manganese was therefore excited with two different photon energies using high flux FEL pulses from the BL2 beamline of FLASH. With photons of 52.1eV (23.8nm) Mn was excited resonantly in its giant resonance, with photons of 61.2eV (20.3nm) non-resonantly above it. m/q spectra were obtained by the means of ion time-of-flight spectrometer depending on the irradiance of the FEL pulses. Charge states of Mn ions up to Mn(6+) have been observed at resonant excitation and even up to Mn(7+) for non-resonant excitation. The dependence of the m/q spectra can be explained in a sequential excitation scheme.

Primary authors:
Dr. KLUMPP, Stephan (DESY) Dr. TIEDTKE, Kai (DESY)

Co-authors :
Dr. MARTINS, Michael (Universität Hamburg) Dr. RICHTER, Mathias (PTB Berlin) Prof. SONNTAG, Bernd (Universität Hamburg) Prof. ZIMMERMANN, Peter (TU Berlin) Ms. KAROLIN, Mertens (Universität Hamburg) Dr. GERKEN, Nils (Universität Hamburg) Dr. BRAUNE, Markus (DESY) Dr. SOROKIN, Andrey (DESY)

Interaction of Highly Charged Ions with Surfaces, Membranes and 2D Materials

Content:

Highly charged ions (HCI) release a large amount of potential energy (the stored ionization energy) when interacting with solids. This energy is deposited into a very small volume via multiple charge exchanges on a fs time scale leading to a highly excited electronic system. Especially ionic crystals have shown a predisposition to potential energy effects due to their low conductivity and their strong electron phonon coupling. On CaF$_2$ surfaces the formation of hillocks induced by the potential energy of a single highly charged Xe^{q+} ion has been observed for charge states higher than $q > 27$. The formation of these hillocks can be attributed to local melting [1]. In contrast, on surfaces of KBr and LiF one monolayer deep pits are formed by defect mediated desorption also showing a threshold behavior in the pit formation [2, 3].
The interaction of HCI with membranes and 2D materials, like graphene, is particularly interesting because the pre-equilibrium interaction regime can be accessed for thicknesses below a few nm. In 1 nm carbon nano membranes (CNM) for instance, holes are produced by the passage of highly charged Xe^{q+} ions [4]. For the formation of these holes a threshold in the potential energy of the HCI exists that depends on the kinetic energy. In order to elucidate the formation mechanism we examined the charge state and the energy loss of the Xe^{q+} ions after their passage through the membrane. Surprisingly, two distinct exit charge distributions were observed [5]. Part of the ions are passing the membrane with almost now charge loss, whereas the other part looses most of their charge. Apparently, the measured charge distribution reflects two different impact parameter regimes. For graphene extremely short charge-equilibration times of a few fs are determined from the mean exit charge state. Additionally, the energy loss of highly charged projectiles is found to be strongly enhanced and to increase quadratically with the incident projectile charge state.

[1] A. El-Said, R. Wilhelm, R. Heller, S. Facsko, C. Lemell, G. Wachter, J. Burgdorfer, R. Ritter, and F. Aumayr, Phys. Rev. Lett. 109, 117602 (2012).
[2] R. Heller, S. Facsko, R.A. Wilhelm, and W. Moller, Phys. Rev. Lett. 101, 096102 (2008).
[3] A.S. El-Said, R.A. Wilhelm, R. Heller, M. Sorokin, S. Facsko, and F. Aumayr, Phys. Rev. Lett. 117, 126101 (2016).
[4] R. Ritter, R.A. Wilhelm, M. Stöger-Pollach, R. Heller, A. Mücklich, U. Werner, H. Vieker, A. Beyer, S. Facsko, A. Gölzhäuser, F. Aumayr, Appl. Phys. Lett. 102, 063112 (2013).
[5] R.A. Wilhelm, E. Gruber, R. Ritter, R. Heller, S. Facsko, F. Aumayr, Phys. Rev. Lett. 112, 153201 (2014).

Primary authors:
Dr. FACSKO, Stefan (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Dr. WILHELM, Richard (Helmholtz-Zentrum Dresden-Rossendorf) Dr. HELLER, René (Helmholtz-Zentrum Dresden-Rossendorf)

Investigation of Large Biopolymer Assemblies using Synchrotron X-ray Radiation

Content:

Proteins fulfill a broad range of different functions in living organisms. Part of their diversity is comprised by triggered self-assembly to macromolecular complexes. The complexes can serve as scaffolds like actin polymers or create new cellular compartments as proteins from the dynamin family by supplying vesicles from membranes.
The human Guanylate Binding Protein 1 (hGBP1) belongs to the family of dynamin-like proteins and its activation is triggered by addition of nucleotides. We are able to show that an isoform of hGBP1 which was used in earlier studies consists of a mixture of monomers, dimers and tetramers after addition of specific nucleotides. By using the natural occurring lipid-modified protein, the protein assembles under same conditions to large polymeric structures. The polymer composition is analyzed in solution using X-ray Small Angle Scattering (SAXS) for determination of the polymerization mechanism and to get insights into the physiological polymer structure.

Primary authors:
Ms. LORENZ, Charlotte (FZ Jülich)

Co-authors :
Mr. STADLER, Andreas (FZ Jülich)

Investigation of lipid layers under pressure and shear as model system for synovial joints

Content:

The unmatched tribological performance of articulated joints is due to both the properties of the cartilage itself and the assumed self-organization of the molecules in the synovial fluid (SF) and at the surface of cartilage. In the synovial tribological system the components of the SF account to different load and shear conditions by re-structuring. Thereby they provide extremely low friction coefficients under low and high pressures up to several hundred bar and shear rates up to 106 s^(-1).
We have investigated the interaction of the components of hyaluronan, lipids and proteins with respect to their arrangement and interaction under shear and pressure. This components form multilayer structures at the interface of the cartilage and it is of great interest how this interfacial structures behave at different load situations and molecular compositions.
Or results show that a smeared layer of HA adsorbs to the lipids. The studies show further that the molecular weight of the biopolymer HA influences strongly the formed structures. Our grazing incidence diffraction measurement (GID), Brewster angle microscopy (BAM) and x-ray reflectivity (XRR) measurements show that the arrangement is not only influence on the micrometer scale but also on the nanometer scale thereby disturbing the lateral packing of the lipids.
Furthermore, we investigated the impact of hydrostatic pressure on the formed structures at the interface by XRR. We could observe that phospholipid bilayers undergo a non-reversible phase transition upon pressure increase. This situation is changed as HA adsorbs to the interface. Composite layers of DPPC/HA showed reversible structural changes. This indicates that HA has a stabilizing effect on the lipid layer structures.

Primary authors:
Dr. WIELAND, Florian (Helmholtz Zentrum Geesthacht)

Co-authors :
Dr. HARAMUS, Vasyl (Helmholtz Zentrum Geesthacht) Prof. WILLUMEIT-RöMER, Regine (Helmholtz Zentrum Geesthacht) Dr. ZANDER, Thomas (Helmholtz Zentrum Geesthacht) Prof. CLASSON, Per (KTH) Dr. DEDINAITE, Andra (KTH)

Investigations of nanogranular systems

Content:

I will present the work performed at DESY in the framework of RT4, materials and nanoscience for information technology. The range spans from novel approaches for nanofocusing of X-ray beams via utilizing advanced self-organization processes for nanostructured organic and metal thin films to in-situ investigations of industrially-relevant nanostructuring processes and operando investigations of functional devices.

Primary authors:
Prof. ROTH, Stephan V. (DESY)

Ion and electron imaging of indole and indole-water

Content:

State-selected, strongly aligned and oriented molecular ensembles serve as ideal samples to study ultrafast chemistry in the molecular frame. Possible probing mechanisms include the investigation of molecular-frame photoelectron angular distributions [1] or the detection of structural changes via X-ray or electron diffraction [2].
We have developed techniques to manipulate the motion of molecules in cold supersonic beams using strong inhomogeneous electric and laser fields at 1 kHz repetition rate [3]. State-selected molecules and clusters are aligned by strong laser fields [4] or oriented in combination of laser fields and static electric fields [5].
Here, reconstructed static three-dimensional molecular frame photoelectron distributions (MFPADs) of indole and its water complex will be presented. They allow the observation of the molecules' electron density distributions, photoelectron kinetic energies, and out-of-molecular-plane emission angles. The experimentally retrieved observables are discussed within an extended strong-field approximation model. It provides a close glimpse at the laser-distorted HOMO potential surfaces of the investigated molecules at the moment of ionization. Furthermore, it allows to determine changes in the polarizability and dipole moment of the neutral and the corresponding ion. In addition, the direct comparison of indole and its 1:1 water complex allows inspection of the nature of hydrogen bonding in biomolecules.
References:
[1] L. Holmegaard et al., Nature Physics, 6, 428 (2010); C. Bisgaard et al., Science 323, 1464–1468 (2009); R. Boll, et al. Phys. Rev. A 88, 061402 (2013).
[2] J Küpper et al, Phys. Rev. Lett 112, 083002 (2014); Filsinger et al., PCCP (diffraction ideas); C. J. Hensley, J. Yang, and M. Centurion, Phys. Rev. Lett. 109, 133202 (2012); Barty, ARPC (2013).
[3] S. Trippel et al., Mol. Phys. 111, 1738 (2013); Y.-P. Chang et al., Int. Rev. Phys. Chem. 34, 557–590 (2015).
[4] H. Stapelfeldt, and T. Seideman, Rev. Mod. Phys., 75, 543–557 (2003).
[5] L. Holmegaard et al, Phys. Rev. Lett., 102, 023001 (2009).

Primary authors:
TRIPPEL, Sebastian (Center for Free-Electron Laser Science, DESY, Hamburg, Germany)

Ion irradiation induced cobalt/cobaltoxide heterostructures: from materials to devices

Content:

Spintronic devices are often patterned from continuous films into micro- or nanostructures. Fabrication of those nano-devices is self-limited and depends on the lateral resolution of the chosen fabrication method. Ion irradiation offers an alternative route to introduce smaller magnetic patterns limited by the size of the ion beam. Irradiation of oxide materials can cause chemical reduction and lead to the local formation of metallic species. By using the oxide family of ferromagnets (e.g., Fe, Ni and Co), reduction leads to the formation of ferromagnetic and conducting volumes limited by the size of the ion irradiated area that are embedded into a non-magnetic and insulating matrix. It was recently demonstrated that local oxide reduction from Co3O4/Pd [1] and CoO/Pd [2] multilayers within nano-patterned regions was possible, leading to well-defined, perpendicularly magnetized volumes. On the other hand, the physical mechanism behind ion irradiation-induced oxide reduction could not be explained. Therefore, our studies focus on ion (H, He, Ne, O) irradiated cobalt-oxide (CoO or Co3O4) systems in order to explain the physics behind the process. Also, the knowledge is being exploited to tune exchange-bias direction, prepare nano contacts for synchronized spin torque oscillators, and to form topographically stabilized magnetic skyrmions.
[1] S. Kim, S. Lee, J. Ko, J. Son, M. Kim, S. Kang, and J. Hong. Nature Nanotechnology, 7:567, 2012.
[2] E. Cho, S. Kim, S. C. Shin, J. Han, J. Shim, R. Shun, J. Hong, and S. Kang. Appl. Phys. Lett., 106:043104, 2015.

Primary authors:
Dr. YILDIRIM, Oguz (Helmholtz-Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research)

Lattice dynamics in ultrathin Ge/Fe3Si/GaAs heterostructures

Content:

Fe3Si is a ferromagnet with TC=566°C, a uniaxial magnetic anisotropy [1] and spin polarization at the Fermi level [2]. These properties combined with the possibility to grow single-crystalline Fe3Si layers on Si, Ge and GaAs established this material as very promising candidate for applications in magnetic, spintronic and logic devices [3].
While the lattice dynamics of bulk Fe3Si have been studied theoretically and experimentally [4,5], we investigated lattice dynamics of Fe3Si nanolayers for the first time. For this purpose Ge/57Fe3Si/GaAs heterostructures with a 57Fe3Si thickness ranging between 2 ML and bulk like films were grown at the Paul-Drude-Institute following a well-established procedure [6]. These layers were capped with Germanium to prevent oxidation of the silicide and to simulate a device-like structure. RHEED and XRR measurements showed films of high crystal quality for all grown samples.
Nuclear inelastic scattering (NIS) was used to measure the phonon density of states (PDOS) of the 57Fe in 57Fe3Si for various film thicknesses. 36 ML 57Fe3Si showed very good agreement with previously made ab-initio phonon calculations for bulk material. Samples with layer thicknesses of 8 ML and 6 ML show less pronounced features at higher energies, whereas the low energy features disappear. For 3 ML layer thickness the PDOS shows a featureless profile. For single crystalline films such a behavior is unexpected and needs further investigation.

S. S. acknowledges the financial support by the Initiative and Networking funds of the President of the Helmholtz Association and the Karlsruhe Institute of Technology (KIT) for the Helmholtz-University Young Investigators Group “Interplay between structure and dynamics in epitaxial rare earth nanostructures” Contract No. VH-NG-625. P. P. and A. M. O. kindly acknowledge support by Narodowe Centrum Nauki (NCN) under Projects No. 2011/01/M/ST3/00738 and No. 2012/04/A/ST3/00331

---

[1] J. Herfort et al., J. Appl. Phys. 103, 07B506 (2008) (2008) [2] A. Ionescu et al., Phys. Rev. B 71, 094401 (2005) (2005)
[3] T. Sadoh et al., Appl. Phys. Lett. 89, 182511 (2006)
[4] S. Dennler and J. Hafner PRB 73, 174303 (2006)
[5] O.G. Randl et al., J. Phys.: Condens. Matter 7, 5983 (1995) [6] B. Jenichen et al., Thin Solid Films 556, 120 (2014)

Primary authors:
Mr. KALT, Jochen (Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany)

Co-authors :
Ms. STERNIK, Małgorzata (Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Kraków, Poland) Dr. SERGEEV, Ilya (Deutsches Elektronen-Synchrotron, D-22607 Hamburg, Germany) Dr. LEUPOLD, Olaf (Deutsches Elektronen-Synchrotron, D-22607 Hamburg, Germany) Mr. PRADIP, Ramu (Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany) Dr. HERFORT, Jens (Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin, Germany) Dr. WILLE, Hans-christian (Deutsches Elektronen-Synchrotron, D-22607 Hamburg, Germany) Dr. PIEKARZ, Przemysław (Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Kraków, Poland) Prof. BAUMBACH, Tilo (Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany) Dr. STANKOV, Svetoslav (Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany)

Lattice dynamics of EuO: an evidence for giant spin-phonon coupling

Content:

Europium monoxide, a semiconducting ferromagnet (Curie temperature = 69 K), has been popular since the early 60s for its giant magneto-optic Kerr [1] and Faraday effects [2]. Recently it has been proposed for an application in the emerging field of spintronics as a source for spin polarized current due to the large exchange splitting of its conduction band [3].
The lattice dynamics of EuO, which is of fundamental importance for the proposed application, is much less known, with only few early Raman studies [4]. Using modern synchrotron methods such as inelastic x-ray scattering (IXS) and nuclear inelastic x-ray scattering (NIS) combined with ab initio phonon calculations we have determined the lattice dynamics of EuO. The IXS experiment revealed that the transverse acoustic phonons at 90 K and below show a remarkable increase of their linewidths towards the Brillioun zone boundary along the Γ-X direction, compared to the room temperature measurements. On the other hand, the LA modes along the same direction as well as the TA and LA modes along Γ-K-X direction remained fairly temperature and momentum independent. With the aid of ab initio calculations, we attribute the observed phenomenon in EuO to a giant momentum and temperature dependent anisotropic spin-phonon coupling.
S.S. acknowledges the financial support by the Initiative and Networking funds of the President of the Helmholtz Association and the Karlsruhe Institute of Technology (KIT) contract VHNG-625. P.P. and A.M.O. acknowledge support by Narodowe Centrum Nauki (NCN) under Projects No. 2011/01/M/ST3/00738 and 2012/04/A/ST3/00331. The financial support of the UHV-Analysis lab via the project KIT-Nanolab@ANKA is acknowledged.

References:
[1] J. H. Greiner and G. J. Fan, Appl. Phys. Lett. 9, 27 (1966).
[2] K. Y. Ahn, J. Appl. Phys. 41, 1260 (1970).
[3] P. G. Steeneken, L. H. Tjeng, I. Elfimov, G. A. Sawatzky, G. Ghiringhelli, N. B. Brookes, and D. J. Huang, Phys. Rev. Lett. 88, 047201 (2002).
[4] R. Pradip, P. Piekarz, A. Bosak, D. G. Merkel, O. Waller, A. Seiler, A.I. Chumakov, R. Rüffer,
A. M. Oles, K. Parlinski, M. Krisch, T. Baumbach, and S. Stankov, Phys. Rev. Lett.116, 185501 (2016)
[5] P. Grünberg, G. Güntherodt, A. Frey, and W. Kress, Phys. B+C 89, 225 (1977); R. Zeyher and W. Kress, Phys. Rev. B 20, 2850 (1979)

Primary authors:
Mr. PRADIP, R (Karlsruhe Institute of Technology)

Co-authors :
Dr. PIEKARZ, P (Institute of Nuclear Physics, Polish Academy of Sciences) Dr. BOSAK, A (European Synchrotron Radiation Facility) Dr. MERKEL, D.g. (European Synchrotron Radiation Facility) Dr. WALLER, O (Karlsruhe Institute of Technology) Dr. SEILER, A (Karlsruhe Institute of Technology) Dr. CHUMAKOV, A.i. (European Synchrotron Radiation Facility) Dr. RüFFER, R (European Synchrotron Radiation Facility) Dr. OLES, A.m. (Marian Smoluchowski Institute of Physics, Jagiellonian University and Max-Planck-Institut für Festkörperforschung) Prof. PARLINSKI, K (Institute of Nuclear Physics, Polish Academy of Sciences) Dr. KIRSCH, M (European Synchrotron Radiation Facility) Prof. BAUMBACH, T (Karlsruhe Institute of Technology) Dr. STANKOV, S (Karlsruhe Institute of Technology)

Lattice dynamics of rare earth silicide nanostructures

Content:

The continuous downscaling of the CMOS devices imposes severe material and processing challenges. This demands a constant search for new self-organizing nanostructures. Among the most critical problems are the quality of interconnects in the circuits, contacts, and the source/drain areas of the transistors. The rare earth silicides became especially attractive for such applications due to their metallic nature and their very low Schottky barrier heights [1-3]. Deposited on Si(001), depending on the thickness and the temperature, some of the lanthanides (Sm, Eu, Dy, Gd, Ho, Er, Yb) self-organize in nanostructures with various morphologies, such as nanowires with high aspect ratios, nanoislands and clusters [4].

We have grown epitaxial $EuSi_2$ films and nanoislands [5] and $DySi_2$ films, nanoislands and nanowires and investigated their lattice dynamics by in situ nuclear inelastic scattering on 151Eu and 161Dy and by first principles calculations. The density of phonon states of the nanoislands and nanowires strikingly deviates from that of the bulk and the surface layers revealing the enormous impact of the confinement effects and interfaces on the atomic vibrations. This manifests itself in a remarkable modification of the thermoelastic properties of the rare-earth silicide nanostructures.

S.S. acknowledges the financial support by the Initiative and Networking funds of the President of the Helmholtz Association and the Karlsruhe Institute of Technology (KIT) for the Helmholtz-University Young Investigators Group "Interplay between structure and dynamics in epitaxial rare-earth nanostructures" contract VH-NG-625. P.P. acknowledges the support by the Polish National Science Center (NCN) under Project No. 2011/01/M/ST3/00738. The European Synchrotron Radiation Facility (ESRF), Grenoble is acknowledged for the synchrotron beamtime at the Nuclear Resonance beamline ID18.

References:
[1] G. L. Molnar et al., J. Appl. Phys. 90, 503 (2001)
[2] M. Ieong et al., Mater. Today 9, 26 (2006)
[3] N. Reckinger et al., Appl. Phys. Lett. 94, 191913 (2009)
[4] J. H. G. Owen et al., J. Mater. Sci. 41, 4568 (2006)
[5] A. Seiler et al., J. Cryst. Growth 407, 74 (2014)

Primary authors:
Dr. STANKOV, Svetoslav (Karlsruhe Institute of Technology)

Co-authors :
Dr. SEILER, Anja (Karlsruhe Institute of Technology) Dr. PIEKARZ, Przemysław (Polish Academy of Sciences) Dr. IBRAHIMKUTTY, Shyjumon (Max Planck Institute for Solid State Research) Dr. MERKEL, Daniel (Hungarian Academy of Sciences) Dr. WALLER, Olga (Karlsruhe Institute of Technology) Mr. PRADIP, Ramu (Karlsruhe Institute of Technology) Dr. CHUMAKOV, Alexander (ESRF-The European Synchrotron) Dr. RüFFER, Rudolf (ESRF-The European Synchrotron) Prof. BAUMBACH, Tilo Gerd (Karlsruhe Institute of Technology) Prof. PARLINSKI, Krzysztof (Polish Academy of Sciences) Prof. FIEDERLE, Michael (University of Freiburg)

Local structure and proton transport in HT-PEFCs measured with neutron scattering

Content:

The conception, design and optimization of fuel cells in general requires a good knowledge of the underlying physical processes on all length scales. In this contribution we focus on High Temperature Polymer Electrolyte Fuel Cells (HT-PEFCs) based on a proton conducting membrane such as poly2,2’-m-(phenylene)-5,5’-bibenzimidazole (PBI) doped with phosphoric acid (PA) and show how microscopic neutron scattering techniques can be related to macroscopic properties of the fuel cell. Contrast variation by using different isotopes and the sensitivity to light elements are the major advantages of neutron scattering. Small angle neutron scattering (SANS) provides insight into the fractal structure of the PA doped membrane on length scales of ~10-500 nm. With quasielastic neutron scattering (QENS), proton diffusion can be measured on local length scales of about 0.1-10 nm [1,2]. The length scale dependent energy transfer measured with QENS gives insight into local proton transport processes in the PBI membrane and in the adjacent electrode layers and allows to relate microscopic proton mobilities with macroscopic measurements, e.g. of the proton conductivity of the membrane [3]. Complementary techniques such as X-ray scattering, TEM or PFG-NMR round up the picture on a broad range of length scales.

[1] Holderer, O. et al, Int. J. Hydrogen Energy, 39, 21657 (2014)
[2] Holderer O., et al, ECS Transactions, 69, 337 (2015)
[3] Majerus, A. et al., ECS Transactions, 50, 1155 (2012)

Primary authors:
Dr. HOLDERER, Olaf (Forschungszentrum Jülich GmbH - JCNS)

Co-authors :
Dr. IVANOVA, Oxana (Forschungszentrum Jülich GmbH - JCNS at MLZ) Dr. KHANEFT, Marina (Forschungszentrum Jülich GmbH - JCNS at MLZ) Dr. HOPFENMüLLER, Bernhard (Forschungszentrum Jülich GmbH - JCNS at MLZ) Dr. LüKE, Wiebke (Forschungszentrum Jülich GmbH - IEK-3) Dr. MAJERUS, Anne (Forschungszentrum Jülich GmbH - IEK-3) Dr. APPAVOU, Marie-sousai (Forschungszentrum Jülich GmbH - JCNS at MLZ) Dr. SZEKELY, Noemi (Forschungszentrum Jülich GmbH - JCNS at MLZ) Dr. KRUTYEVA, Margarita (Forschungszentrum Jülich GmbH - JCNS) Dr. ZORN, Reiner (Forschungszentrum Jülich GmbH - JCNS) Prof. LEHNERT, Werner (Forschungszentrum Jülich GmbH - IEK-3, RWTH Aachen University, Faculty of Mechanical Engineering)

MD Simulations of Star Polymers - a look at Branch Point Motion to Investigate Dynamic Tube Dilution and the Role of Functionality

Content:

Large-scale molecular dynamics simulations of three-arm and four-arm symmetric as well as asymmetric star polymers have been performed to study the motion of the branch point. The effect of Dynamic Tube Dilution (DTD) as well as the role of functionality can be investigated by this method. The simulated star polymer systems consist of three- and four-arm stars. Asymmetric stars with a short unentangled third side arm were also simulated, all using standard bead spring models. DTD is a constraint-release mechanism: the inner segments close to the branchpoint probe a tube that broadens with time, since entanglements with outer segments (that have relaxed at much earlier time scales) are not effective. Therefore, for a given observation time window, the effect of DTD will be more relevant the shorter the arms are. This will be demonstrated by the simulation results and with Neutron Spin Echo (NSE) measurements [1]. Functionality, i.e., the number of arms stemming from the branch point, drastically challenges the tube model as a standard approach for describing entangled branched polymers. On the one hand, the mobility of the branch point may be enhanced through more channels for "diving modes". This non-constraint-release mechanism describes excursions of the branch point into the different tubes of the arms and leads to tube broadening [2]. On the other hand, higher functionality results in an increase in the local density of entanglements around the branch point, which may lead to tube narrowing and a reduction in mobility of the branch point. The change in mobility induced by the former two mechanisms manifests itself in a change in the plateau height of the dynamic structure factor. In our simulations we observed a decrease in mobility with higher functionality for all systems, suggesting dominant tube narrowing. These simulations form the basis for future NSE spectroscopy measurements that we expect to further support our findings.

[1] M. Zamponi, W. Pyckhout-Hintzen, A. Wischnewski et al., Macromolecules 43 (2010) 518.
[2] P. Bacova, L.G.D. Hawke, D.J. Read, A.J. Moreno, Macromolecules 46 (2013) 4633.

Primary authors:
Mr. HOLLER, Stefan (FZ Jülich)

Co-authors :
Mr. MORENO, Angel (Centro de Fisica de Materiales) Ms. ZAMPONI, Michaela (FZ Jülich)

MML RT3 Materials and Processes for Energy and Transport Technologies @ DESY

Content:

I will present recent advances in the field of in-situ and operando observations of materials under conditions relevant for energy storage and conversion as well as synthesis of novel materials.

Primary authors:
Prof. STIERLE, Andreas (DESY)

Magnetic Structure of Atomically Exchange Biased Dy20Co80 Film

Content:

Amorphous Rare-Earth - 3d Transition Metal alloys (RE-3d TM) are fascinating magnetic materials due to the easy, straight-forward tunability of their magnetic properties, depending on temperature and concentration ratio between the RE and 3d TM components. If the RE-3d TM alloy is made up of heavier RE, both elements will be antiferromagnetically coupled by an atomic exchange interaction and show a temperature dependent resulting magnetization influenced by the different behavior of both sites. For DyxCo100-x, it results into a transition from the Dy to a Co dominant magnetic phase with increasing temperature where the compensation temperature between both sites can be adjusted by the concentration ratio between both elements1,2. A novel atomic exchange bias3 was found in a thin Dy20Co80 film of about 50 nm resulting in a wing hysteresis loop with the origin of the loop shifted by 4 T. The analysis of detailed xray magnetic circular dichroism (XMCD) measurements traced back the effect to different surface and bulk magnetic configurations of surface and bulk. The occurrence of the wing shaped hysteresis loops shows that the surface and the bulk are strongly magnetically coupled by the atomic exchange interaction keeping the two magnetic states stable in a certain magnetic field range and suggest a non-collinear magnetic configuration in the intersection. The surface contribution dominates at higher fields and couples the magnetization of the bulk via the Zeeman interaction into the same direction, at lower fields, the bulk part dominates and the surface contribution is coupled via atomic exchange interaction with the bulk. For gaining precise qualitative and quantitative information about both competitive interactions, information about the magnetic structure of the film and its internal coupling behavior is required as it cannot be extracted from XMCD data. Polarized neuron reflectometry (PNR) is ideally suited to investigate the magnetic depth profile of the film. The polarization analysis of the reflected neutron beam enables one to detect the depth dependent orientation of the magnetization in Dy20Co80 film, in particular to trace the expected non-collinear configuration in the region between surface and bulk. Moreover, an in-depth analysis of PNR spectra taken at different temperatures allows to gain further information about the switching process and thus to monitor the changes in the magnetization profile that leads to the intriguing exchange bias effect observed in the system.

[1] A. Agui et al., Journal of Physics and Chemistry of Solids 68, (2007) 2148-2152.
[2]Chen, K., Lott, D. et al.. Phys. Rev. B 91, 024409 (2015)
[3] Chen, K., Lott, D. et al. "Observation of an atomic exchange bias effect in DyCo4 film", Sci. Rep. 5,
18377; doi: 10.1038/srep18377 (2015).

Primary authors:
Ms. HOFBAUER, Inken (HZG)

Co-authors :
Dr. CHEN, Kai (University of Cologne) Dr. MATTAUCH, Stefan (Jülich Centre for Neutron Science, Garching, Germany) Dr. LOTT, Dieter (HZG)

Magnetism in EuFe2As2-based Iron Pnictides: Complementary Neutron and X-ray Studies

Content:

Doped EuFe2As2 is a unique representative of the 122 type family of iron based superconductors due to the two magnetic sublattices and the strong coupling between spin-, lattice- and charge degrees of freedom. This talk will give an overview about our recent experimental results on the static magnetism in doped EuFe2As2 compounds, investigated by neutron and resonant x-ray diffraction.

Primary authors:
Dr. JIN, Wentao (Juelich Center for Neutron Science at MLZ, Forschungszentrum Juelich GmbH)

Co-authors :
Dr. XIAO, Yinguo (Juelich Center for Neutron Science, Forschungszentrum Juelich GmbH)
Dr. SU, Yixi (Juelich Center for Neutron Science at MLZ, Forschungszentrum Juelich GmbH)
Prof. BRUECKEL, Thomas (Juelich Center for Neutron Science, Forschungszentrum Juelich GmbH)

Magnon Transport in Spin Textures

Content:

One of the grand challenges in cutting edge quantum and condensed matter physics is to harness the spin degree of electrons for information technologies. While spintronics, based on charge transport by spin polarized electrons, made its leap in data storage by providing extremely sensitive detectors in magnetic hard-drives, it turned out to be challenging to transport spin information without great losses. With magnonics a visionary concept inspired researchers worldwide: Utilize magnons - the collective excitation quanta of the spin system in magnetically ordered materials - as carriers for information. Magnons are waves of the electrons' spin precessional motion. They propagate without charge transport and its associated Ohmic losses, paving the way for a substantial reduction of energy consumption in computers.

While macroscopic prototypes of magnonic logic gates have been demonstrated, I envision magnonics going beyond wave-based information processing: I believe, that the future of magnonics lies in the combination of magnons with nano-sized spin textures. Both magnons and spin textures share a common ground set by the interplay of dipolar, spin-orbit and exchange energies rendering them perfect interaction partners. Magnons are fast, sensitive to the spins' directions and easily driven far from equilibrium. Spin textures are robust, non-volatile and still reprogrammable on ultrashort timescales. The vast possibilities offered by combining this toolset of magnetic phenomena, add value to both magnonics and the fundamental understanding of complex spin textures.

Novel materials exhibiting spin textures predestined for manipulating magnons are just being discovered. In this presentation I will give an introduction about magnon propagation and manipulation in non-collinear spin textures with an outlook towards future experiments.

Primary authors:
Dr. SCHULTHEISS, Helmut (HZDR)

Metal Nanoparticles on Graphene

Content:

Small metal nanoparticles have gained increasing interest in surface science because of their widespread applications, especially in heterogeneous catalysis.
It was previously shown that physical vapor deposition of selected elements on a graphene/Ir(111) template leads to the formation of ordered cluster arrays.
With this approach monodisperse clusters with diameters smaller than 2 nm and a very high surface coverage can be grown.

In this contribution, we compare the atomic structure of small metal clusters made of Pt, Rh, Pt/Rh and Ir/Pd by means of surface x-ray diffraction and discuss the adsorption behaviour of CO on Pt, Rh and Pt-Rh alloy nanoparticles on graphene/Ir(111) using vibrational spectroscopy under UHV conditions. The metal nanoparticles are deposited at room temperature and the CO adsorption is investigated below 170 K.

SXRD measurements benefit enormously from the coherent signal enhancement of the ordered metal clusters, so that the atomic structure of these small metal clusters (shape, lattice parameter, stacking) and the element distribution of bimetallic clusters can be determined.

The UHV-IRRAS data demonstrate one CO adsorption site for small Pt and Rh nanoparticles, which is assigned to on-top edge sites of the nanoparticles, while for larger clusters the adsorption of CO on-top edge sites is only preferred at low CO coverages. For higher CO coverages a second (additional) adsorption site with higher wavenumbers is observed, which is interpreted as on-top adsorption sites on nanoparticle terrace atoms.

Primary authors:
Mr. CREUTZBURG, Marcus (DESY FS-NL) Mr. FRANZ, Dirk (DESY FS-NL)

Co-authors :
Dr. NOEI, Heshmat (DESY FS-NL) Prof. STIERLE, Andreas (DESY FS-NL)

Microstructure development and mechanical strength of transient liquid phase bonded gamma-TiAl alloy joints

Content:

TiAl alloys are increasingly used as light weight material in aero engines, which also leads to a demand for repair methods. Transient liquid phase bonding is a promising method to close cracks (in noncritical or not highly loaded areas) in parts made of TiAl alloys. Here two brazing alloys based on Ti-Fe and Ti-Ni are used for brazing Ti-45Al-5Nb-0.2B-0.2C (in at. %).
The phases and their distribution in the brazing zone were determined at room temperature after bonding by high-energy X-ray diffraction (HEXRD) using the materials science beamline HEMS at the PETRA III synchrotron radiation facility at DESY in Hamburg, Germany. Additionally, measurements were performed time and space resolved during the bonding process. Furthermore, tensile tests were performed at room temperature showing different strengths depending on the brazing alloy.
In addition, analysis with electron microscopy and electron backscatter diffraction (EBSD) show significantly different grain sizes in the joint regions for the two types of brazing alloys. These results can be combined with the analysis of the development of the phase constitutions over bonding time in the joint region with HEXRD. With this we can explain the different development of the microstructures and thus the different mechanical strength.

Primary authors:
HAUSCHILDT, Katja (Helmholtz-Zentrum Geesthacht)

Co-authors :
STARK, Andreas (Helmholtz-Zentrum Geesthacht) SCHELL, Norbert (Helmholtz-Zentrum Geesthacht) PYCZAK, Florian (Helmholtz-Zentrum Geesthacht) MüLLER, Martin (Helmholtz-Zentrum Geesthacht)

Microstructure of gas atomized TiAl powders

Content:

Due to the rapid development of advanced additive manufacturing production routes in recent years, the demand of high quality alloy powders is significantly increased. We studied gas-atomised spherical powders of several Nb-bearing γ-TiAl based alloys, Ti-45Al-10Nb and Ti-45Al-5Nb-xC in at.% (x = 0, 0.5, 0.75, and 1), which were produced in-house by HZG using the plasma melting induction guided gas atomization (PIGA) technique. The phase composition of different powder fractions was determined by synchrotron high-energy X-ray diffraction at the HEMS beamline P07 at PETRA III (DESY), as well as by SEM, EDX, 2D and FIB based 3D EBSD measurements. Due to the high cooling rates in the range of 1·104 K/s, the powder particles mainly consist of hexagonal-close-packed α- and body-centred-cubic β-phase. As the cooling rate depends on the particle size, considerable amounts of the β phase only were found in the small powder fractions. The total β phase amount was generally higher in the alloy with a higher Nb content, and also the effect of carbon, known as a strong α-stabilizer, was observed. Dendritic cauliflower-like structures are more pronounced in bigger powder particles due to the slower solidification and thus a higher Nb segregation in the remaining melt. The absence of preferred misorientation angles between α-grains indicates that α-grains are not formed out of already solidified β-grains by a solid state phase transformation.

Primary authors:
LAIPPLE, Daniel (Helmholtz-Zentrum Geesthacht)

Co-authors :
WANG, Li (Helmholtz-Zentrum Geesthacht) RACKEL, Marcus (Helmholtz-Zentrum Geesthacht) STARK, Andreas (Helmholtz-Zentrum Geesthacht) SCHWEBKE, Bernd (Helmholtz-Zentrum Geesthacht) PYCZAK, Florian (Helmholtz-Zentrum Geesthacht) SCHREYER, Andreas (Helmholtz-Zentrum Geesthacht)

Molecular dynamics investigated with free-electron lasers

Content:

Free-Electron Lasers, such as FLASH or LCLS, enable completely new experiments in the XUV to hard X-ray spectral range by providing extremely short light pulses with very high peak intensities. These unique properties allow studying time-resolved processes with multi-photon x-ray absorption in (gas phase) atomic and molecular systems. High-Z constituents (e.g. iodine in halogenated hydrocarbons) can serve as markers within the molecule to create well localized centers of absorption and to study ultra-fast charge rearrangement in small to medium-sized molecular systems. By combining this technique with femtosecond UV laser pulses we can control the internuclear distance between the iodine and its molecular environment and follow charge transfer as a function of distance. Using hard x-ray pulses with intensities exceeding 10^19 W/cm^2, we studied the charge rearrangement in iodomethane and iodobenzene upon multiphoton x-ray absorption producing charge states up to 47+.

Primary authors:
Dr. ERK, Benjamin (DESY)

NMR spectroscopy of frustrated quantum spin systems at highest magnetic fields

Content:

Nuclear magnetic resonance (NMR) spectroscopy in pulsed magnetic fields up to the regime of 70 Tesla and beyond is now routinely available as a user instrument at the Dresden High Magnetic Field Laboratory. This powerful experimental method is a unique research tool for the investigation of strongly correlated states of matter in highest magnetic fields. As an example application, we present recent experimental results of the strongly frustrated quantum magnet strontium-copper-borate, which give microscopic evidence of
the 1/3 magnetization plateau, in agreement with findings from thermodynamic observables.

This work was done in collaboration with R. Stern (NICPB, Estonia), J. Kohlrautz and J. Haase (University of Leipzig), E.L. Green, Z.T. Zhang, T. Herrmannsdörfer, and J. Wosnitza (HZDR Dresden), as well as H.A. Dabkowska and B.D. Gaulin (McMaster University, Canada).

Primary authors:
Dr. KüHNE, Hannes (Hochfeld-Magnetlabor Dresden / Helmholtz-Zentrum Dresden-Rossendorf)

Nano-optical 3D devices for advanced X-ray instrumentation

Content:

The objectives of the HZB team in the reporting POF III period are addressed to science and technology of nano-optical devices for advanced synchrotron radiation instrumentation and methods with cutting-edge spatial and temporal resolution. with. HZB has developed,fabricated and tested nano-optical elements of three types:
 The 3-dimentional and quasi-three dimensional reflection zone plates for implementation in spectroscopy and monochromatization of synchrotron and free electron laser beams. [1-3]
 Development of 3-dimentional high efficiency multilayer coated blazed gratings. [4]
 Development of active acousto-optical X-ray elements with ultra-high temporal resolution. [5-7]
All above mentioned nano-optical elements and devices have been successfully tested with synchrotron and X-ray laser radiation at BESSY II, LCLS, ALS and DIAMOND facilities. The special instrumentation for optical tests has been built at the BESSY II facility [8].
References
1.Femtosecond high-resolution hard X-ray spectroscopy using reflection zone plates, H. Löchel, C. Braig, M. Brzhezinskaya, F. Siewert, P. Baumgärtel, A. Firsov, Optics Express, 23 (7), (2015), 8788-8799
2.Hard x-ray spectroscopy and imaging by a reflection zone plate in the presence of astigmatism, C. Braig, H. Löchel, A. Firsov, M. Brzhezinskaya, A. Hafner, J. Rehanek, M. Wojcik, A. Macrander, L. Assoufid, and A. Erko, Optics Letters , 41(1), (2016), 29-32
3.X-ray absorption spectroscopy using a self-seeded soft X-ray free-electron laser, Th. Kroll, J. Kern, M. Kubin, D. Ratner, S. Gul, F. D. Fuller, H. Löchel, J. Krzywinski, A. Lutman, Y. Ding, G. L. Dakovski, S. Moeller, J. J. Turner, R. Alonso-Mori, D. L. Nordlund, J. Rehanek, C. Weniger, A. Firsov, M. Brzhezinskaya, R. Chatterjee, B. Lassalle-Kaiser, R. G. Sierra, H. Laksmono, E. Hill, A. Borovik, A. Erko, A. Föhlisch, R. Mitzner, V. K. Yachandra, J. Yano, P. Wernet, U. Bergmann, Optics Express, (2016), 24(20), 22469-22480
4.Highly efficient blazed grating with multilayer coating for tender X-ray energies, F. Senf, F. Bijkerk, F. Eggenstein, G. Gwalt, Q. Huang, R. Kruijs, O. Kutz, S. Lemke, Louis, E.; M. Mertin, I. Packe, I. Rudolph, F. Schäfers, F. Siewert, A. Sokolov, J. M. Sturm, Ch. Waberski, Z. Wang, J. Wolf, T. Zeschke, A. Erko, Optics Express (2016) 24(12) 13220-13230
5.Surface acoustic wave propagation in graphene film, D. Roshchupkin, L. Ortega, I. Zizak, O. Plotitcyna, V. Matveev, O. Kononenko, E. Emelin, A. Erko, K. Tynyshtykbayev, D. Irzhak and Z. Insepov, J. Appl. Phys. 118, 104901 (2015).
6.Piezoelectric Ca3NbGa3Si2O14 crystal: crystal growth, piezoelectric and acoustic properties, D. Roshchupkin, L. Ortega, O. Plotitcyna, A. Erko, I. Zizak, S. Vadilonga, D. Irzhak, E. Emelin, O. Buzanov, W. Leitenberger, Applied Physics A (2016) 122:753
7.Observation of sagittal X-ray diffraction using surface acoustic waves in Bragg geometry, S. Vadilonga, I. Zizak, D. Roshchupkin, E. Emelin, A.Petsiuk, W. Leitenberger A. Erko, Journal Applied Crystallography, to be published, 2017
8.The at-wavelength metrology facility for UV- and XUV-reflection and diffraction optics at BESSY-II, F. Schäfers, P. Bischoff, F. Eggenstein, A. Erko, A. Gaupp, S. Künstner, M. Mast, J.-S. Schmidt, F. Senf, F. Siewert, A. Sokolov and Th. Zeschke, J. Synchrotron Rad. (2016). 23, 67–77

Primary authors:
Prof. ERKO, Alexei (Helmholtz Zentrum Berlin)

Nanoscale rheology of phospholipid membranes

Content:

We present a novel approach to measure fluctuations of molecular structures close to a solid interface. As an example we show results of membrane dynamics of phospholipid (L-α-phsophatidylcholin, SoyPC) membranes on a solid substrate (silicon), extracting local interaction and friction parameters. This is achieved by Grazing Incidence Neutron Spin Echo Spectroscopy (GINSES), where an evanescent neutron wave probes the fluctuations in the sample close to a rigid interface. Here we access length scales in the nano- to micrometer region and energies on the order of μeV . Only by using a new neutron resonator structure we achieved the required intensity gain for this experiment. The observed modes of these biological membranes can provide a dissipation mechanism for energy which helps stabilizing them. This new methodology has the capability to probe the viscoelastic effects contributing to lubrication and thus become a new tool for tribology on the nanoscale.

Primary authors:
Dr. JAKSCH, Sebastian (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ)

Co-authors :
Dr. HOLDERER, Olaf (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ) Mr. GVARAMIA, Manuchar (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ) Dr. OHL, Michael (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ) Dr. MONKENBUSCH, Michael (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ) Dr. FRIELINGHAUS, Henrich (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ)

Nanotomography at the P05 beamline

Content:

The Imaging Beamline IBL/P05 at the DESY storage ring PETRA III, operated by the Helmholtz-Zentrum Geesthacht, has two dedicated endstations optimized for micro- and nanotomography experiments. Here we present the status of the nanotomography endstation, highlight the latest instrumentation upgrades and present first experimental results.
In particular in materials science, where structures with ceramics or metallic materials are of interest, X-ray energies of 15 keV and above are required. Even for sample sizes of several 10 µm in diameter lower energies are often not feasible. The P05 nanotomography instrument is dedicated to materials science and is designed to allow for imaging applications with X-ray energies of 10 to 50 keV. In addition to the commissioned full field X-ray microscopy setup the highly flexible layout of the endstation allows switching to cone-beam configuration. Kinematics for X-ray optics like CRLs, Fresnel zone plates, beam-shaping optics are implemented and a KB-mirror system can also be installed into the optics hutch. Altogether this leads to a high flexibility of the nanotomography setup such that the instrument can be tailored to the specific requirements of the sample system.

Primary authors:
Dr. GREVING, Imke (HZG)

Co-authors :
Dr. OGURRECK, Malte (Diamond light source) Dr. WILDE, Fabian (HZG) BURMESTER, Hilmar (HZG) DOSE, Thomas (HZG) LOTTERMOSER, Lars (HZG) Prof. MUELLER, Martin (HZG) Dr. BECKMANN, Felix (HZG)

Nanotubes, Nanocones and Nanotube Networks Fabricated by Ion-Track Technology and ALD of TiO2, SiO2, and Al2O3

Content:

Synthetic nanopores and nanotubes attract wide attention due to possible applications in the fields of nanofluidics, filtration, catalysis, and sensorics. Tailoring of single nanopores with nanometric diameters enables the mimicking of ion channels in biological cell membranes. Also, synthetic single-pore membranes have great potential as single-molecule sensors and devices for molecular recognition.
At the GSI Helmholtz Center in Darmstadt, polymer foils are irradiated with MeV - GeV heavy ions. The irradiation conditions can be adjusted to vary the ion density between one single ion per sample up to ~1011 ions/cm2 [1]. By chemical etching each ion track is selectively dissolved and enlarged into a nanopore with well-controlled diameter. Atomic layer deposition (ALD) is applied for conformal modification of the pore surface and tailored decrease of the pore diameter to a few nanometers.
In this work, 30 µm thick polycarbonate membranes were employed to produce series of single- and multi-pore membranes with various pore diameters between 18 and 55 nm. After surface modification by ALD, homogeneity, conformity, and composition of the coatings (SiO2, Al2O3 and TiO2) inside the nanopores were investigated. Small angle x-ray scattering before and after ALD showed conformal coating along the full pore length. X-ray photoelectron spectroscopy evidenced nearly stoichiometric composition of the different coatings. By wet-chemical methods, the ALD-deposited films were released from the supporting polymer templates providing 30 µm long self-supporting nanotubes with walls as thin as 5 nm. Electrolytic ion-conductance measurements provided proof-of-concept that combining ALD coating with ion-track nanotechnology offers promising perspectives for single-pore applications by controlled shrinking of an oversized pore to a preferred smaller diameter and fine-tuning of the chemical and physical nature of the inner channel surface [2].

[1] M.E. Toimil-Molares, Beilstein J Nanotechnol 2012, 3, 860-83, DOI:10.3762/bjnano.3.97
[2] A. Spende et al. Nanotechnology 2015, 26(33), 335301, DOI:10.1088/0957-4484/26/33/335301

Primary authors:
CARRILLO SOLANO, Mercedes Alicia (Materials Research, GSI Helmholtz Center for Heavy Ion Research)

Co-authors :
ULRICH, Nils (Materials Research, GSI Helmholtz Center for Heavy Ion Research, Material- und Geowissenschaften,Technische Universität Darmstadt, Darmstadt, Germany) SPENDE, Anne (Materials Research, GSI Helmholtz Center for Heavy Ion Research, Material- und Geowissenschaften,Technische Universität Darmstadt, Darmstadt, Germany) Prof. TRAUTMANN, Christina (Materials Research, GSI Helmholtz Center for Heavy Ion Research, Material- und Geowissenschaften,Technische Universität Darmstadt, Darmstadt, Germany) TOIMIL-MORALES, Maria Eugenia (Materials Research, GSI Helmholtz Center for Heavy Ion Research)

Narrowband inverse Compton scattering x-ray sources at high laser intensities

Content:

Inverse Compton Scattering (ICS) is a valuable source of X- and gamma-rays for various applications in medicine, materials science and nuclear physics. Main advantage of ICS sources is their ability to provide a very narrow bandwidth (<1%) photon spectrum, albeit with a very low conversion efficiency. One way to dramatically increase the total photon yield, is to increase the laser photon density, i.e. increase the laser pulse peak intensity. Unfortunately, scattering laser pulse intensity is strongly limited by the fact that the generated spectrum can be nonlinearly broadened due to the ponderomotive force, and a bandlike structure can appear in the fundamental frequency as well as its harmonics even for rather low values of laser pulse amplitude.

In this contribution, analytical and numerical results of photon energy-angular spectrum calculations for the case of the nonlinear ICS are presented. It is demonstrated, that the nonlinear broadening can be mitigated by appropriately choosing the laser pulse frequency chirp. Results are valid both using purely classical and QED calculations.

Primary authors:
Dr. RYKOVANOV, Sergey (Helmholtz Institute Jena)

Co-authors :
Dr. KHARIN, Vasily (Helmholtz Institute Jena) Dr. SEIPT, Daniel (Cockcroft Institute, Daresbury, UK)

Near surface structure and dynamics using neutron scattering

Content:

A sensitivity about structures and dynamics in the normal direction close to surfaces is obtained by grazing incidence (GI) neutron scattering experiments. The static structures are obtained by GI small angle neutron scattering (GISANS), while the dynamics are obtained by GI neutron spin-echo spectroscopy (GINSES). All these methods need to deal with low intensities due to small footprints and small scattering volumes. For this purpose, we developed a neutron resonator. Using constructive interference, the wave field intensity in the sample can be enhanced manyfold.
Scientific examples display the need for near-surface characterizations. And the development of the tools for enhanced intensities are presented.

Primary authors:
Dr. FRIELINGHAUS, Henrich (Forschungszentrum Jülich GmbH, JCNS at MLZ)

Neutron Imaging of Hydrogen Storage Tanks

Content:

Hydrogen is a promising energy carrier for the future, especially for mobile applications. It can be stored safely and reversibly at high volumetric densities in hydrogen storage tanks filled with light metal hydrides.
Due to the sensitivity of neutrons towards hydrogen, in situ Neutron Radiography (NR) is the ideal technique for time-resolved investigations of the hydrogenation process of metal hydride powder beds and pellets inside a hydrogen storage tank. Neutron Computerized Tomography (NCT) provides additional 3D information about the material structure and hydrogen distribution.
While low and medium temperature hydrides [1,2] have already been studied by NR and NCT, first-time in situ NR measurements of a hydrogen storage tank filled with the high-temperature complex hydride LiBH4-MgH2 at NECTAR and ANTARES beamlines at FRM II have been performed. Combining cold and fission neutron spectra of both instruments and using a new method for the quantitative investigation of neutron imaging data [3,4], a precise study of the hydrogen distribution in this high-temperature hydride is possible. Effects of temperature field and material packing density were investigated and the 3D struture was analysed additionally by NCT. The results allow for optimizing the hydrogen storage tank filled with metal hydride powder in terms of capacity, kinetics and safety.

[1] P. K. Pranzas et al., Advanced Engineering Materials 13 (8) (2011), 730-736
[2] Bellosta von Colbe, J.M. et al.; Int. Journal of Hydrogen Energy 37 (2012), 2807
[3] S. Börries et al., Scattering influences in quantitative fission neutron radiography for the in situ analysis of hydrogen distribution in metal hydrides, NIM A 797 (11) (2015), 158
[4] S. Börries et al., Optimization and comprehensive characterization of metal hydride based hydrogen storage systems using in-situ Neutron Radiography, Journal of Power Sources 328 (2016), 567

Primary authors:
Dr. PRANZAS, P. Klaus (HZG)

Co-authors :
Mr. BöRRIES, Stefan (HZG) Mr. METZ, Oliver (HZG) Dr. BüCHERL, Thomas (Institut für Radiochemie der TU München) Dr. SöLLRADL, Stefan (Siemens Healthcare GmbH) Dr. BELLOSTA VON COLBE, José (HZG) Dr. DORNHEIM, Martin (HZG) Prof. KLASSEN, Thomas (HZG) Prof. SCHREYER, Andreas (European Spallation Source ERIC) Prof. MüLLER, Martin (HZG)

Neutron scattering investigation of the effect of active principles on phospholipid-based membranes.

Content:

Phospholipid-based bilayers are widely used as model systems for studying the more complicated biological cell membranes, providing information about their structure and interactions. In particular, we are interested in understanding the effect of drugs on phospholipid-based membranes, i.e. the action mechanism, and the eventual toxicity when administered at high concentrations. This knowledge can in principle support a chemical design of more efficient variants having lower side effects.
In the present study, we have investigated the effect of some active principles, namely benzocaine and propranolol on bilayers composed of L-α-phosphatidylcholine (SoyPC) by means of Neutron Reflectivity (NR) and Small Angle Neutron Scattering (SANS).
Benzocaine is a commercial drug that serves as topical pain reliever, used for instance in cough drops. It is also found as main component in many anesthetic ointments such as products for oral ulcers. Propranolol is a beta-blocker, affecting the heart and blood circulation: it is used for treating tremors, angina, hypertension and other heart or circulatory conditions. We generally found a variation of the structural parameters of the membranes with incorporated drug molecules, with a destabilization found at high drug concentrations, through the formation of ruptures inside the double layers, randomly distributed over the space. Propranolol has a bigger perturbative effect on the membranes, due to the structure of his hydrophobic part.
Keywords: neutron reflectivity, small angle neutron scattering, phospholipid, cell membranes

Primary authors:
Mr. MANUCHAR, Gvaramia (Juelich Centre for Neutron Science)

Co-authors :
Dr. MANGIAPIA, Gaetano (juelich center of neutron scattering) Dr. FRIELINGHAUS, Henrich (juelich center of neutron scattering) Mr. KUHRTS, Lucas (Applied physical chemistry, TU Berlin)

Neutron scattering to study the structure and dynamics of macromolecules

Content:

In this talk, a number of key results obtained in Jülich Centre for Neutron Science on structure and dynamics of macromolecules investigated by neutron scattering will be presented. In first part, the importance of macromolecular topology on the dynamics and very recent insights into the structure and dynamics of ring polymers will be discussed [1,2]. In the next part I will talk about dynamics of polymeric matrix in nanocomposites. In particular, influence of the polymer-surface interaction on the polymer dynamics and specific phase formation will be addressed [3]. Later a combined analysis of small-angle neutron scattering (SANS), linear rheology and pulsed field gradient (PFG) NMR spectroscopy experiments on the supramolecular association and chain structure of well-defined telechelically modified poly(ethylene glycol) (PEG) in the bulk will be presented. Moreover, based on the static results [4], the dynamical NSE experiment directly reveal hydrogen bond lifetime, which is one of the key parameters determining macroscopic properties of supramolecular polymer melts [5]. Finally, the investigation of the hydrogen- bonding mechanism in a transiently branched comb-like polymer system in the melt is reported [6]. The rheology data corroborate the SANS evidence of a dominant heterocomplementary association, leading to the formation of a transient comb structure.

[1] S. Gooßen et al., Phys. Rev. Letters 113, 168302 (2014)
[2] S. Gooßen et al., Phys. Rev. Letters 115, 148302 (2015)
[3] M. Krutyeva et al., Phys. Rev. Letters 110, 108303 (2013)
[4] Krutyeva, M. et al., Macromolecules 48, 8933 (2015)
[5] Monkenbusch, M.; Krutyeva, M. et al., Phys. Rev. Letters 117, 147802 (2016)
[6] Staropoli, M.; Raba, A.; Hövelmann, C.; Krutyeva, M. et al., Macromolecules 49 (15), 5692 (2016)

Primary authors:
Dr. KRUTYEVA, Margarita (Forschungszentrum Jülich GmbH)

New results for the structure of certain warm dense matter states

Content:

The dynamic and static structure factors contain a wealth of information about the state and properties of a physical system. The structure of a system relates directly to its equation of state, collective modes, stopping power and relaxation processes. Since x-ray and particle scattering are extremely important experimental tools to diagnose warm dense matter, theoretical predictions of the structure have become one of the best modes of comparison between theory and experiment in the warm dense matter regime.

We give an overview of state of the art theoretical methods to calculate the structure of warm dense matter in equilibrium and non-equilibrium. Results are given for such states as created in recent experiments. Limits of the current theories and possible future developments are discussed.

Primary authors:
Dr. VORBERGER, Jan (HZDR)

Nitrogen doping in niobium (100) single-crystal

Content:

Ranging from particle physics to material science, medicine and industry, Superconducting Radio Frequency (SRF) particle accelerators are keystones of modern research. These facilities rely on niobium RF cavities for their operation and there is a big drive for performance improvement of such cavities. Increasing the acceleration gradient and achieving a higher efficiency Q0, the so-called quality factor, will lead to higher luminosity while reducing the dynamic heat load, resulting in potential cost savings and lower energy consumption. Nitrogen doping is known to increase the performance of niobium cavities [1], however, the physical and chemical processes and phenomena involved are far from understood [1,2]. In this work, niobium (100) single-crystals were subjected to a recently proposed nitrogen selvedge doping preparation, which is coined ‘nitrogen infusion’ [3]. This process consists of 800°C annealing for two hours in high vacuum followed by annealing at 120°C in nitrogen atmosphere for 23 hours. The changes in the surface layers were monitored by in-situ X-Ray Reflectivity (XRR) measurements, while the presence of nitride, oxide or oxy-nitride phases of niobium were investigated by ex-situ Grazing Incidence X-Ray Diffraction (GIXRD), X-Ray Photoemission Spectroscopy (XPS) and Scanning Electron Microscopy (SEM). The results show a decrease in the thickness of the native niobium oxide upon high-temperature annealing and the formation of an approximately 15nm thick niobium nitride layer during the nitrogen-infusion.

[1] A. Grassellino et al, Supercond. Sci. Technol. 26 102001 (2013).
[2] P. Dhakal et al, IEEE Tran. on App. Superc. 25 3500104 (2015).
[3] Solyak N. et al, ECFA linear collider workshop (2016).

Primary authors:
Mr. DALLA LANA SEMIONE, Guilherme (Deutsches Elektronen-Synchrotron DESY; Fachbereich Physik Universität Hamburg)

Co-authors :
Ms. DANGWAL PANDEY, Arti (Deutsches Elektronen-Synchrotron DESY) Mr. VONK, Vedran (Deutsches Elektronen-Synchrotron DESY) Mr. STIERLE, Andreas (Deutsches Elektronen-Synchrotron DESY; Fachbereich Physik Universität Hamburg)

Nuclear spin effects in water and ammonia

Content:

Water is the third most common molecule in the Universe. Detailed interpretation of the properties of this apparently small and simple molecule is one of the important open problems in the molecular sciences. The complexity of ice and liquid water represents tremendous scientific challenges and at the moment are not readily explained in terms of standard models. Ammonia is one of the principal deposits of nitrogen molecules. Its chemical properties and a characteristic large-amplitude inversion motion, associated with the double-well potential, together with its practical importance, have made ammonia a prototype system for many molecular studies.
Water and ammonia both exist in two nuclear-spin-isomer forms, ortho and para, which correspond to different magnitudes of the molecule's overall nuclear spin due to the hydrogen nuclei. The ortho and para spin states can be treated as though they were different molecules, which are associated one-to-one with different rovibronic levels in the molecule. Little is known about the mechanism that converts the two nuclear spin isomers in general, and even less for the process in isolated molecules. One possible way to study the conversion is to analyze the strongly forbidden transitions between rovibrational energy levels belonging to different spin isomers. There is a huge number of rovibrational transitions in the spectra of water and ammonia and preliminary theoretical analysis of the strongest transitions is highly demanding.
Here we present a first accurate calculation of the hyperfine structure in the rovibrational spectra of ammonia and its fully deuterated isotopologue. The rovibrational line lists have been computed variationally using the program suite TROVE, a new spectroscopically determined potential energy surface and ab initio quadrupole, spin-spin, and spin-rotation coupling surfaces. The line lists cover transitions between levels with rotational excitations up to J = 20 and vibrational band centers up to 8000 cm-1 above zero point energy. Comparisons with experimental data confirm high accuracy of the computed results which is essential for modeling Doppler limited high resolution spectra. The perspectives of spectroscopic observation of the ortho-para conversion, for instance using infrared frequency comb spectroscopy, and its modulation by external electric field are discussed.

Primary authors:
Dr. YACHMENEV, Andrey (CFEL) Prof. KüPPER, Jochen (CFEL)

Observation of sagittal diffraction of x-rays by surface acoustic waves in Bragg geometry.

Content:

Meridional diffraction of X-ray beams on surface acoustic waves (SAWs) was demonstrated previously in several works [1,2]. X-ray Bragg diffraction in sagittal geometry on the Y-cut of langasite crystal (La3Ga5SiO14) modulated by a $\Lambda = 3$ μm Rayleigh surface acoustic waves was studied at the BESSY II synchrotron radiation facility. To excite SAWs an interdigital transducer (IDT) made of Aluminum was deposited on the surface of LGS crystal. Due to the crystal lattice modulation by the surface acoustic wave diffraction the satellites appear. Their intensity and angular separation depends on the amplitude and wavelength of the ultrasonic super-lattice. Experimental results are compared with the corresponding theoretical model that exploits the kinematical diffraction theory. This experiment shows that the propagation of the surface acoustic waves creates a dynamical diffraction grating on the crystal surface, and this can be used for space-time modulation of an X-ray beam.

References
[1] D.V. Roshchupkin et al., Applied Physics A, 114 (2014)
[2] R. Tucoulou et al., Nuclear Instruments and Methods in Physics Research B 132, 207-213 (1997)

Primary authors:
Mr. VADILONGA, Simone (Helmholt Zentrum berlin)

Co-authors :
Dr. ZIZAK, Ivo (Helmholt Zentrum berlin) Mr. PETSIUK, Andrei (Helmholtz Zentrum Berlin) Prof. ERKO, Alexei (Helmholt Zentrum berlin) Dr. ROSHCHUPKIN, Dmitri (IMT RAS)

Oxidation behaviour of arc evaporated (Ti,Cr,Al)N coatings studied by SR-XRPD

Content:

Hard and wear resistant cubic (c)-(Ti,Al)N based coatings have many applications, such as protection of the underlying bulk material and improved wear resistance. In the cutting tool industry, the improved wear resistance increases the lifetime of the coated tools. The mechanical properties of TiAlN deteriorates at high temperatures due to formation of the hexagonal (h) AlN phase, while by alloying of Cr in (Ti,Al)N coatings the detrimental effect of h-AlN on the mechanical properties can be reduced. Further, the oxidation resistance of CrAlN coatings is improved compared to that of TiAlN, thus, a TiCrAlN coating could be expected to have both, high oxidation resistance and high mechanical properties. In this study, in-situ high-energy synchrotron radiation x-ray powder diffraction (SR-XRPD) during annealing in an air atmosphere has been performed to study the oxidation process of TiCrAlN. The results reveal that the oxidation behavior changes with Al-content and Ti-content and TiCrAlN with low Ti-content show a higher oxidation resistance.

Primary authors:
Mr. OSTACH, Daniel (Helmholtz Zentrum Geesthacht)

Co-authors :
Dr. SCHROEDER, Jeremy (Thin Film Physics, Department of Physics, Chemistry and Biology (IFM), Linköping University) Mr. CHEN, Yu-hsiang (Nanostructured Materials, Department of Physics, Chemistry and Biology (IFM), Linköping) Dr. ROGSTRØM, Lina (Nanostructured Materials, Department of Physics, Chemistry and Biology (IFM), Linköping University) Dr. GHAFOOR, Naureen (Nanostructured Materials, Department of Physics, Chemistry and Biology (IFM), Linköping University) Dr. JOHANSSON-JõESAAR, Mats (R Material and Technology Development, SECO Tools AB, SE-737 82 Fagersta) Dr. SCHELL, Norbert (Helmholtz Zentrum Geesthacht) Prof. BIRCH, Jens (Thin Film Physics, Department of Physics, Chemistry and Biology (IFM), Linköping University) Prof. SCHREYER, Andreas (Helmholtz Zentrum Geesthacht)

PM2 – A new soft x-ray beamline for magnetism

Content:

The BESSY II dipole beamline PM2 has recently been built as a state-of-the-art instrument for the investigation of magnetism in condensed matter samples by soft x-ray radiation. Polarization switching within 2 seconds and energy scans in fly-mode allow most efficient data acquisition. Measurements of x-ray magnetic circular and linear dichroism benefit from the excellent signal-to-noise ratio. Current studies concentrate on magnetic dynamic and in-equilibrium phenomena in thin film samples and at interfaces, magnetic nanostructures and magnetic molecules. These studies aim at a broader understanding of future spintronic devices.

Primary authors:
Dr. RYLL, Hanjo (Helmholtz-Zentrum Berlin)

Co-authors :
BALZER, Andreas (Helmholtz-Zentrum Berlin) DRESCHER, Lars (Helmholtz-Zentrum Berlin) EGGENSTEIN, Frank (Helmholtz-Zentrum Berlin) FLEISCHHAUER, Roland (Helmholtz-Zentrum Berlin) KALUS, Christian (Helmholtz-Zentrum Berlin) PAWLIZKI, Olaf (Helmholtz-Zentrum Berlin) Prof. RADER, Oliver (Helmholtz-Zentrum Berlin) RINGEL, Rudolf (Helmholtz-Zentrum Berlin) RUDORFF, Steffen (Helmholtz-Zentrum Berlin) SCHMIDT, Jan-simon (Helmholtz-Zentrum Berlin) SULJOTI, Ervis (Helmholtz-Zentrum Berlin) Dr. RADU, Florin (Helmholtz-Zentrum Berlin)

PRIOR - a protom microscope for FAIR

Content:

A prototype of the PRIOR (Proton Microscope for FAIR) facility has been recently constructed and successfully commissioned at GSI using 3.5-4.5 GeV intense proton beams from the SIS-18 synchrotron. The PRIOR-I setup has been fielded at the HHT area of GSI and it employs high-gradient (120 T/m) NdFeB permanent magnet quadrupole (PMQ) lenses. The static commissioning of PRIOR-I has demonstrated 30 μm spatial resolution with remarkable density sensitivity. For dynamic commissioning, a new pulsed power generator (50 kV, 10 μF) has been constructed and installed at HHT for underwater electrical wire explosion experiments. During the dynamic commissioning run, 0.8 mm diameter exploding (180 kA, 1.3 μs rise time) Ta wires have been radiographed by PRIOR-I using 3.6 GeV proton beam. A temporal resolution of 5–10 ns has been achieved and the expansion of the Ta plasma at different specific power deposition levels up to 10 GW/g has been compared with optical measurements.
The PRIOR-I commissioning experiments have also indicated that the PMQ lenses are not an appropriate choice for the final design of the PRIOR facility due to the severe radiation damage of the PQM magnets. Therefore the final design of the PRIOR proton microscope (PRIOR-II) employs small but strong and radiation-resistant electromagnets (60 mm aperture and 1.3 T pole tip field). The PRIOR-II design assumes that the setup will be first fielded at the HHT area of GSI to use up to 4 GeV protons delivered by the SIS-18 synchrotron for static or dynamic experiments, and later will be transferred without modifications to the new experimental area at FAIR and used with intense 2–5 GeV proton beams of the SIS-100 synchrotron. The PRIOR-II facility will provide a magnification of about 3.5 at GSI and up to 8 at FAIR with 10 μm spatial resolution at the object. The first experiments with the PRIOR-II facility at GSI are planned for the end of 2018.

Primary authors:
Dr. BLAZEVIC, Abel (GSI)

Polythiophene Based Block Copolymers for Neutron Scattering

Content:

Deuterium labeled compounds have gained an enormous importance in neutron science due to the different scattering length densities of deuterium (2H or D) compared to hydrogen (1H). In neutron scattering experiments this difference allows contrast variation leading to information about structure and dynamics of molecules which is not accessible by other methods such as X-ray scattering. While deuterated small molecules are often easily accessible, deuterated polymers need in many cases elaborated synthetic strategies starting with monomer synthesis. Especially, a pre-defined molecular weight and narrow molecular weight distribution are highly desired. This contribution shows exemplarily the synthesis of a block copolymer consisting of Poly-3-hexylthiophene (P3HT) and Polyethylene oxide (PEO) with a focus on reaction design, synthetic difficulties, evaluation of block-connecting methods and polymer characterization.

Primary authors:
Dr. RABA, Andreas (Forschungszentrum Juelich)

Co-authors :
Dr. ALLGAIER, Jürgen (Forschungszentrum Juelich) Dr. FRIELINGHAUS, Henrich (Forschungszentrum Juelich)

Probing dynamics in colloidal crystals with pump-probe experiments at LCLS

Content:

I will present results of the studies of dynamics in colloidal crystals performed by pump-probe experiments at LCLS. Colloidal crystals are attractive for multiple applications since they can be used as large-scale low-cost templates to fabricate novel materials with unique optical properties such as the full photonic bandgap, ’slow’ photons and negative refraction. In our experiment colloidal crystals were pumped with the infrared (IR) laser at 800 nm wavelength with the varying power and probed with the time delay up to 1000 ps by the XFEL pulses at energy of 8 keV. The positions of the Bragg peaks, their radial and azimuthal widths were analyzed as a function of time delay.

Primary authors:
Ms. MUKHARAMOVA, Nastasia (DESY)

Co-authors :
Dr. LAZAREV, Sergey (DESY) Dr. VARTANYANTS, Ivan (DESY) Mr. GOROBTSOV, Oleg (DESY) Mr. DZHIGAEV, Dmitry (DESY)

Probing multi-functional Oxides with scattering techniques

Content:

Complex transition-metal oxides are often correlated electron systems with ordering tendencies of electronic degrees of freedom (charge, orbital, spin) potentially leading to functionalities interesting for applications. Functional oxides include for example magnetoelectric multiferroics, which have a large applications potential in information technology. Suitable mechanisms of multiferroicity encompass ferroelectricity driven by charge order (CO) and spin order (SO), both of which are highly suited for investigations by scattering methods. SO-driven ferroelectricity involves naturally a very strong magnetoelectric coupling. Ferroelectricity arising from CO is also expected to yield large magnetoelectric coupling as the same ions are involved in both CO and SO.
Rare earth ferrites had long been considered the prototypical “proof-of-principle” examples and have correspondingly attractted a lot of attention [2]. However, the CO in $LuFe_2O_4$, determined with scattering techniques [3], turned out to be non-polar, and previous macroscopic indications of ferroelectricity have been explained in terms of extrinsic effects. We have recently focused on $YbFe_2O_4$ and YFe_2O_4. The former behaves very similar to $LuFe_2O_4$, which may be expected based on a very similar rare earth ion size. However, a subtle modification of the CO superstructure at low temperature points to a distinct CO, refined in P-1. The much larger ion size of YFe_2O_4, on the other hand leads to completely different CO, with two distinct CO phases, the refinement of which is discussed. The ion size effect is further investigated by studying partially substituted $Y_xLu_{1-x}Fe_2O_4$. All CO phases found so far are centrosymmetric.
Classical magnetite both shows macroscopic indications of at least relaxor ferroelectricity and possesses a polar CO crystal structure [4]. Our time-resolved diffraction data confirm a structural response to voltage-pulses consistent with ferroelectric switching, proving the intrinsic nature of ferroelectricity in magnetite.

[1] See, e.g., T. Mueller, J. de Groot, J. Strempfer, and M. Angst, J. Crystal Growth 428, 40 (2015).
[2] For recent reviews see M. Angst, Phys. Status Solidi RRL 7, 383 (2013); N. Ikeda, T. Nagata, J. Kano, and S. Mori, J. Phys.: Condens. Matter 27, 053201 (2015).
[3] J. de Groot, T. Mueller, R.A. Rosenberg, D.J. Keavney, Z. Islam, J.-W. Kim, and M. Angst, Phys. Rev. Lett. 108, 187601 (2012).
[4] M.S. Senn, J.P. Wright, and J.P. Attfield, Nature 481, 173 (2012).

Primary authors:
Prof. ANGST, Manuel (Forschungszentrum Juelich GmbH)

Co-authors :
Ms. WILLIAMSON, Hailey (Forschungszentrum Juelich GmbH) Mr. MUELLER, Thomas (Forschungszentrum Juelich GmbH) Ms. ADIGA, Shilpa (Forschungszentrum Juelich GmbH) Dr. GORFMAN, Semen (Universität Siegen) Dr. STREMPFER, Jörg (Deutsches Elektronen Synchrotron DESY) Prof. BALAKRISHNAN, Geetha (University of Warwick) Ms. HAMMOUDA, Sabreen (Forschungszentrum Juelich GmbH)

Propagation based X-ray phase contrast and 4D in vivo imaging of development in Xenopus laevis

Content:

We present results on micron and 20min resolved 4D development in Xenopus laevis (gastrulation, neurulation). The imaging modality is propagation based X-ray phase-contrast micro-tomography.

Primary authors:
Mr. TROST, Fabian (IPS KIT)

Co-authors :
Dr. HOFMANN, Ralf (IPS KIT) Prof. BAUMBACH, Tilo (IPS KIT)

Proton Disorder in D2O – Ice: A Neutron Diffraction Study

Content:

K. Siemensmeyer1, J.-U. Hoffmann1, S. V. Isakov2, B. Klemke1, R. Moessner3, J. P. Morris4, D. A. Tennant5

1Helmholtz-Zentrum Berlin, Hahn Meitner Platz 1, D-14109 Berlin, Germany
2 Google, Brandschenkestrasse 110, 8002 Zürich, Switzerland
3 Max Planck Institut für Physik komplexer Systeme, D-01187 Dresden, Germany
4 Xavier University, Cincinnati, OH 45207, USA
5 Neutron Sciences Directorate, ORNL, Oak Ridge TN 37831, USA

Water ice (H2O) at low pressure can be understood as a hexagonal structure where each Oxygen atom is bound to two Hydrogen atoms. Further, each bond between Oxygen atoms is occupied by only one Hydrogen atom. These are the famous ice - rules that give rise to a highly disordered ground state with a residual entropy of R Ln(3/2). We have measured the diffuse scattering from a large D2O – ice crystal using neutron diffraction. Different to previous descriptions of the ice - structure by Monte Carlo methods we are able to explain the data using an analytical method: The structure is mapped to a divergence-free dipolar model which is solved within a large-N approach. We obtain remarkable agreement between model and neutron results. The correlation length obtained at T = 30 K seems to be finite which is surprising at such low temperature.

References:
[1] Analytical theory for proton correlations in common water ice Ih, S. V. Isakov, R. Moessner, S. L. Sondhi, D. A. Tennant, Phys. Rev. B91, 245152 (2015)
[2] Electromagnetism on ice: classical and quantum theories of proton disorder in hexagonal water ice, O. Benton, O. Sikora, N. Shannon, arXiv 1504.04158

Primary authors:
Dr. SIEMENSMEYER, Konrad (Helmholtz-Zentrum Berlin)

Pump-Probe Holographic Imaging of Nanoscale Magnetic Domains

Content:

While ultrafast magnetization dynamics of homogeneously magnetized samples has been studied by optical pump-probe techniques since decades [1], it is still an open question in research on magnetism how nanoscale magnetic domain patterns react to an ultrashort optical stimulus. Only with the advent of free-electron lasers it has become possible to probe the nanoscale on the relevant sub-picosecond time scale [2]. Here, we report on an IR-pump–FEL-probe imaging experiment on a (0.4nm Co/0.2nm Pd)x30 multilayer deposited on a silicon nitride membrane. The multilayer exhibits a perpendicular magnetic anisotropy and a disordered maze-domain pattern with a domain size in the range of 80 nm. The other side of the silicon nitride membrane has been covered with an opaque gold film and an object hole and reference holes were milled into the gold film to enable Fourier transform holography (FTH) measurements [3]. The experiment was conducted at DiProI beamline at FERMI@Elettra using FEL radiation tuned resonantly to the M absorption edge of cobalt, i.e., a wavelength of 20.8 nm. By using FTH, the real-space domain configuration can be directly retrieved unambiguously by applying a Fourier transform to the scattering data. We fixed the pump-probe delay time to 1 ps and followed the evolution of the domain pattern at different pump fluences. The image contrast, which is proportional to the sample's saturation magnetization, significantly decreases with pump fluence and vanishes at a high fluence of 16.3 mJ/cm², hence, revealing ultrafast demagnetization on the nanoscale. Further, at moderate fluences (8.2 mJ/cm²), we observed a spatial change, namely a rearrangement of the maze domains, that happens on time scales much larger than the delay time of 1 ps. This behavior is due to quasi-static heating of the sample accompanying the exposure with a repetition rate of 10 Hz [4].

[1] E. Beaurepaire, J. Merle, A. Daunois, and J. Bigot, Phys. Rev. Lett. 76, 4250 (1996).
[2] L Müller, S. Schleitzer, C. Gutt, B. Pfau, et al., Sync. Rad. News 26(6), 23 (2013).
[3] S. Eisebitt, J. Lüning, W.F. Schlotter, M. Lörgen, et al., Nature 432, 885 (2004).
[4] L. Müller, C. Gutt, S. Streit-Nierobisch, et al., Rev. Sci. Instrum. 84, 013906 (2013).

Primary authors:
Dr. PHILIPPI-KOBS, André (DESY) SCHLEITZER, Stefan (DESY) Dr. MüLLER, Leonard (DESY) Dr. BERNTSEN, Magnus H. (KTH Royal Institute of Technology) Dr. ROSEKER, Wojciech (DESY) Dr. GEILHUFE, Jan (Helmholtz-Zentrum Berlin für Materialien und Energie) Prof. EISEBITT, Stefan (Helmholtz-Zentrum Berlin für Materialien und Energie) Prof. GRüBEL, Gerhard (DESY)

Co-authors :
Prof. GUTT, Christian (Universität Siegen) Dr. GAUTIER, J. (ENSTA Paris Tech-CNRS) Dr. PFAU, Bastian (TU Berlin) Dr. WEDER, David (TU Berlin) Dr. VON KORFF SCHMISING, Clemens (TU Berlin) Dr. VODUNGBO, Boris (ENSTA Paris Tech-CNRS) Dr. LI, K. (Université Pierre et Marie Curie) Dr. MALINOWSKI, G. (Université Paris-Sud) Dr. TUDU, B. (Université Pierre et Marie Curie) Dr. CAPOTONDI, Flavio (Elettra-Sincrotone Trieste) Dr. PEDERSOLI, Emanuele (Elettra-Sincrotone Trieste) Dr. KISKINOVA, Maya (Elettra-Sincrotone Trieste) Prof. LüNING, Jan (Université Pierre et Marie Curie)

Quantitative characterization of degradation processes in situ by means of a bioreactor coupled flow chamber under physiological conditions using time-lapse SRµCT

Content:

Magnesium and its alloys are used increasingly in implant materials research as their good biocompatibility and biodegradability suggest a high potential for clinical application. In order to prove their use it is pivotal to understand the degradation processes taking place under physiological conditions. The techniques traditionally used in degradation research are mainly two-dimensional and destructive, thus yielding only localized and overall averaged information. The processes occurring during degradation are however highly complex and spatially variable, thus necessitating a time-resolved, three-dimensional analysis. To this end, we have applied time-lapse synchrotron radiation micro-computed tomography (SRµCT) to study the degradation of a Mg2Ag pin in Minimum Essential Medium alpha (α MEM, Life Technologies, Germany) in a custom-built corrosion cell in situ over five days. Imaging was performed at beamline P05 at the PETRA3 storage ring of the Hamburger Synchrotronstrahlungslabor (HASYLAB), Deutsches Elektronen-Synchrotron (DESY), with a spatial resolution of 2.5 µm. For the analysis the image data was segmented using the Fiji (Schindelin et al., 2012) plugin WEKA trainable segmentation (Arganda-Carreras et al., 2016). Subsequently, the data was radially resliced and analysed using Matlab ® R2016a (The MathWorks Inc., USA). The degradation rate after five days of the bulk magnesium determined from SRµCT data agreed with values obtained by in vitro immersion tests (Myrissa et al., 2016). The 3D nature of the images allowed identification of regions of H2 development and resulting cracks in the degradation product layer, as well as the shrinkage of the overall sample surface over time. The image data can further be utilized for image-based modelling to simulate the occurring processes and to deepen the understanding of the mechanisms of magnesium degradation.

ARGANDA-CARRERAS, I., KAYNIG, V., RUEDEN, C., SCHINDELIN, J., CARDONA, A. & SEUNG, H. S. 2016. Trainable_Segmentation: Release v3.1.2.
MYRISSA, A., AGHA, N., LU, Y., MARTINELLI, E., EICHLER, J., SZAKACS, G., KLEINHANS, C., WILLUMEIT-ROMER, R., SCHAFER, U. & WEINBERG, A. 2016. In vitro and in vivo comparison of binary Mg alloys and pure Mg. Materials Science & Engineering C-Materials For Biological Applications, 61, 865-874.
SCHINDELIN, J., ARGANDA-CARRERAS, I., FRISE, E., KAYNIG, V., LONGAIR, M., PIETZSCH, T., PREIBISCH, S., RUEDEN, C., SAALFELD, S., SCHMID, B., TINEVEZ, J. Y., WHITE, D. J., HARTENSTEIN, V., ELICEIRI, K., TOMANCAK, P. & CARDONA, A. 2012. Fiji: an open-source platform for biological-image analysis. Nature Methods, 9, 676-682.

Primary authors:
ZELLER-PLUMHOFF, Berit (Department of Metallic Biomaterials, Helmholtz-Zentrum Geesthacht)

Co-authors :
FEYERABEND, Frank (Department of Metallic Biomaterials, Helmholtz-Zentrum Geesthacht) DOSE, Thomas (2Department of Materials Physics, Helmholtz-Zentrum Geesthacht) WILDE, Fabian (2Department of Materials Physics, Helmholtz-Zentrum Geesthacht) HIPP, Alexander (2Department of Materials Physics, Helmholtz-Zentrum Geesthacht) HAMMEL, Jörg (Department of Materials Physics, Helmholtz-Zentrum Geesthacht) BECKMANN, Felix (Department of Materials Physics, Helmholtz-Zentrum Geesthacht) WILLUMEIT-RöMER, Regine (Department of Metallic Biomaterials, Helmholtz-Zentrum Geesthacht)

RT4@DESY

Content:

A status report of the current activities of the different groups participating in RT4 at DESY will be given.

Primary authors:
Prof. ROTH, Stephan V. (DESY)

Radial growth of self-catalysed GaAs nanowires probed by time-resolved in-situ high-resolution X-ray diffraction

Content:

Philipp Schroth1,2,3, Julian Jakob2,3, Martin Köhl3, Ludwig Feigl3, Seyed Mohammad Mostafavi Kashani1, Jonas Vogel1, Arman Davtyan1, Jörg Strempfer4, Tilo Baumbach2,3 and Ullrich Pietsch1

1) Universität Siegen, Siegen, Germany
2) Laboratory for Application of Synchrotron Radiation (LAS), Faculty of Physics, Karlsruhe Institute of Technology
3) Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
4) Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany

Time-resolved X-ray measurements can provide valuable insight in the dynamics of the growth of semiconductor nanostructures as e.g. GaAs nanowires, in particular in the evolution of their crystallographic properties and their shape. Here, we report on the growth of self-catalysed GaAs nanowires onto Silicon (111) substrates using the portable molecular beam epitaxy setup of LAS/IPS1 at KIT. These nanowires are grown by the vapour-liquid-solid mode using a liquid Ga-droplet as catalyst. We probe the crystallographic properties and the shape of the growing nanowires in-situ by means of time-resolved high-resolution X-ray diffraction.
The X-ray experiments have been performed at the P09 beamline of PETRA III at DESY. We gain insight in the evolution of polytypism in self-catalyzed GaAs nanowires during growth. Further, we obtain information on radial growth processes of wurtzite and zinc-blende segments in the growing GaAs nanowires. In particular, we separate radial facet growth processes from tapering caused by an inflation of the liquid Ga droplet and compare the findings with ex-situ SEM and theoretical growth models.

Acknowledgements

We are grateful for Thomas Keller and Andreas Stierle at the Nanolab@DESY, David Reuther at P09, Hans Gräfe, Bärbel Krause and Annette Weißhardt at the UHV-laboratory@ANKA, KIT. The project was supported by German BMBF (05ES7CK and 05K13PS3).

References:

1T. Slobodskyy, et al., Rev. Sci. Instrum. 83, 105112 (2012).

Primary authors:
Mr. SCHROTH, Philipp (Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology)

Re-association dynamics of supramolecular transient networks

Content:

Supramolecular polymers form an emerging class of tailor-made materials as they offer enhanced tuneable properties due to their re-associating groups. The thus introduced novel motifs such as shape memory or self-healing are found in diverse applications, e.g. sensors, shock absorbers or coatings, where precise control of the molecular properties is required. For the rational design of these novel smart materials a fundamental understanding of the underlying physical processes is essential.

We present a multiple methods investigation into the dynamics of entangled supramolecular polyisoprene networks with the objective, to decipher the so far unexplained gross discrepancy between transient bond life times and rheological relaxation. Structural information from neutron small angle scattering (SANS) shows a homogenous supramolecular melt, with functionalized chains displaying a Gaussian conformation. Independent information on the association constant of the functional H-bonding groups is revealed by Fourier Transformed Infrared Spectroscopy (FTIR). In the common temperature range the H-bond lifetime (dielectric α*-process) and the rheological relaxation due to the supramolecular stickers differ by two orders of magnitude in time.

Within the concept of a compact random walk, where the random walker (urazole group acting as a sticker) undergoes multiple returns to its starting point, we quantitatively understand the so far unexplained discrepancy between rheological and dielectric relaxation: The bond dissociation gives rise to the dielectric response. However, for mechanical relaxation, the association with a new partner, taking place only after multiple returns to the original binding partner, is relevant.

Primary authors:
GOLD, Barbara (JCNS-1, Forschungzentrum Jülich)

Co-authors :
Dr. PYCKHOUT-HINTZEN, Wim (JCNS-1, Forschungzentrum Jülich) Dr. ALLGAIER, Jürgen (JCNS-1, Forschungzentrum Jülich) Dr. WISCHNEWSKI, Andreas (JCNS-1, Forschungzentrum Jülich) Prof. RICHTER, Dieter (JCNS-1, Forschungzentrum Jülich)

Recent Developments on Etched Ion-Track Membranes for Sensor Applications

Content:

In the past decades, polymer etched ion-track membranes have been widely used for applications in filtration, surface protection, and life sciences, and as templates for the formation of nanowires and nanotubes [1]. Their fabrication involves two separate processing steps: (i) Irradiation of the template material with swift heavy ions and creation of latent tracks; (ii) selective ion-track dissolution and formation of channels by chemical etching. Control over the irradiation and etching conditions enables the production of various membranes with channels of predefined geometries, sizes and aspect ratios [1,2].

More recently, single etched ion-track membranes have been developed and characterized as nanofluidic diodes. Currently, efforts are being particularly devoted to develop surface modification techniques that confer specific surface functionalities to the nanochannels [3].

In this talk, we will present recent results obtained on the surface modification of etched ion-track membranes by atomic layer deposition (ALD) [4]. By ALD, we have successfully and conformally coated membranes with few nm thin SiO_2, TiO_2, and Al_2O_3 layers. The coatings have been characterized by scanning electron microscopy after dissolution of the polymer template in an organic solvent. Figure 1 shows representative images of the resulting cylindrical and conical tubes, as well as nanotube networks. Ionic transport studies of cylindrical and conical single nanochannels before and after ALD will be discussed, explaining in particular how the isoelectric point of the deposited surface layer affects the ionic transport at different pH values. In addition, recent examples of polymer-based nanochannel sensors based on different surface modification methods will be discussed.

[1] C. Trautmann, Particle Acceleration and Detection Ion Beams in Nanoscience and Technology 2010, p. 369-387 R. Hellborg, H. J. Whitlow and Y. Zhang Springer Berlin Heidelberg
[2] M.E. Toimil-Molares, Beilstein J. of Nanotechnology 3 (2012) 860.
[3] G. Perez-Mitta, C. Trautmann, M.E. Toimil-Molares, O. Azzaroni, Single ion track-etched nanochanels for analytical applications, in Chemically modified nanopores and nanochannels, Ed. By M. Tagliazucchi and I. Szleifer (2016)
[4] A. Spende et al. Nanotechnology 26 (2015) 335301.

Primary authors:
Dr. TOIMIL-MOLARES, Maria Eugenia (GSI Helmholtz Centre for Heavy Ion Research)

Co-authors :
Dr. SPENDE, Anne (GSI Helmholtz Centre for Heavy Ion Research) Mr. ULRICH, Nils (GSI Helmholtz Centre for Heavy Ion Research) Prof. TRAUTMANN, Christina (GSI Helmholtz Centre for Heavy Ion Research)

Relativistic calculations of the non-resonant two-photon K-shell ionization of neutral atoms

Content:

The non-resonant two-photon one-electron K-shell ionization of neutral atoms is studied within the framework of relativistic second-order perturbation theory and independent particle approximation. The importance of relativistic and screening effects in the total as well as differential cross sections is investigated. Our results show that, at near two-photon ionization threshold energies, the account for the screening effects of the remaining electrons leads to occurrence of an unexpected minimum in the total two-photon ionization cross section and to elliptical dichroism in the photoelectron angular distribution. For ionization of heavy atoms, relativistic effects result in a significant decrease of the total cross section, and in distortion of the angular distribution into forward direction.

Primary authors:
Mr. HOFBRUCKER, Jiri (Helmholtz Institute Jena)

Co-authors :
Dr. VOLOTKA, Andrey (Helmholtz Institute Jena) Prof. FRITZSCHE, Stephan (Helmholtz Institute Jena)

Requirements for stoichiometric SrCoO3_3-delta thin films

Content:

Transition metal oxides are a big research topic, because they offer a wide range of possible applications, particularly in information and energy technology [1]. One such system is strontium cobaltite (SrCoO_3-delta), which exists in two distinct topotactic phases, depending on the oxygen content. SrCoO_3 is a ferromagnetically ordered metal with a Curie temperature of 305 K, but the system becomes an antiferromagnetic insulator with a Néel temperature of 570 K, when the oxygen content is decreased to SrCoO_2.5. Along with this magnetic transition, the structure changes from perovskite to the orthorhombic brownmillerite, with the missing oxygen atoms forming vacancy channels.

We aim at growing thin films of strontium cobaltite via molecular beam epitaxy. This method offers the possibility to control the stoichiometry of the sample by varying the deposition rate of the individual elements. To prepare a film of the desired stoichiometry, the growth conditions have to be calibrated.

The goal is to determine the growth parameters to achieve a sample stoichiometry of SrCoO_3, to optimize the growth of the perovskite structure with a low surface roughness and to investigate the magnetic properties of the stoichiometric samples. To this end, multiple sample series at a specific Co rate were grown, while varying the Sr rate. The growth rates were determined with a quartz crystal micro-balance. Rutherford backscattering measurements were performed to determine the stoichiometry and to correlate the Co:Sr growth rates with the stoichiometry. Initial measurements revealed an abundance of Co, so the rates were adjusted to compensate. The samples were characterised in-situ with low energy electron diffraction (LEED) and reflection high energy electron diffraction and ex-situ with x-ray reflectivity and atomic force microscopy. Obviously, the surface roughness decreases with approaching the correct stoichiometry. Most of the samples show crystallinity in LEED.

In our poster session, we focus on a comprehensive overview of the samples addressing the requirement to achieve the correct stoichiometry.

[1] J. Zhang and R.D. Averitt, "Dynamics and Control in Complex Transition Metal Oxides", doi: 10.1146/annurev-matsci-070813-113258

Primary authors:
Mr. SCHöFFMANN, Patrick (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85747 Garching, Germany)

Co-authors :
Dr. PüTTER, Sabine (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85747 Garching, Germany) Dr. SCHUBERT, Jürgen (Peter Grünberg Institute, PGI-9: Semiconductor Nanoelectronics, JARA: Fundamentals of Future Information Technologies, Forschungszentrum Jülich, Leo-Brandt Straße 1, 52425 Jülich, Germany) Mr. ZANDER, Willi (Peter Grünberg Institute, PGI-9: Semiconductor Nanoelectronics, JARA: Fundamentals of Future Information Technologies, Forschungszentrum Jülich, Leo-Brandt Straße 1, 52425 Jülich, Germany) Dr. HELLER, Réne (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01328 Dresden, Germany) BRüCKEL, Thomas (Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH)

Sample environments for x-ray tomography at PETRA III beamline P05.

Content:

The P05 beamline at PERTA III in Hamburg, operated by the Helmholtz-Zentrum Geesthacht (HZG), is dedicated to x-ray tomography and consists of two experimental end stations: a nano tomography end station and a micro tomography end station. Here, we report on available sample environments at the P05 micro tomography end station. The micro tomography end station was designed to provide ample space for sample environments. Apart from existing HZG provided sample environments it is easy and encouraged to implement user sample environments. A selection of user provided sample environments will also be presented.

Primary authors:
Dr. WILDE, Fabian (Helmholtz-Zentrum Geesthacht)

Co-authors :
Dr. HAMMEL, Jörg U. (Helmholtz-Zentrum Geesthacht) Mr. DOSE, Thomas (Helmholtz-Zentrum Geesthacht) Dr. TOLNAI, Domonkos (Helmholtz-Zentrum Geesthacht) Dr. BECKMANN, Felix (Helmholtz-Zentrum Geesthacht) Dr. SKET, Federico (IMDEA Materials)

Self-assembly of periodic nanostructure arrays based on ion-induced spontaneous surface nanopatterning

Content:

Nanopatterning of different materials is a key requirement in research fields as diverse as magnetism, plasmonics, optics or catalysis. Potential technological applications range from photovoltaics augmented by light trapping [1] to high-sensitivity biomolecule detection using plasmonic signal enhancement [2] and high-speed low-energy information encoding, transmission, and processing based on magnonic crystals [3]. Industrial-scale fabrication of such devices for energy harvesting, medical diagnostics, or information technology requires nanopatterning processes which are fast, facile, cost-effective, scalable, and highly reproducible. A versatile bottom-up nanopatterning approach which can meet these demands is based on ion irradiation of semiconductor surfaces and well-established thin film deposition techniques.

On crystalline semiconductor substrates, nanoscale surface patterns with well-defined lateral periodicity form via the mechanism of reverse epitaxy, i.e. the non-equilibrium self-assembly of vacancies and ad-atoms under ion irradiation [4]. The GaAs(001) surface exhibits highly uniform faceting and therefore lends itself to transferring this pattern regularity to other materials. The nanopatterned GaAs surface can for instance be employed as a substrate for molecular beam epitaxy under grazing incidence, producing arrays of nanodots, nanowires, periodically corrugated thin films, or combinations thereof by geometrical shading. It can also be the basis for hierarchical self-assembly: here, the topography of the GaAs surface provides a preferential direction for the chemical microphase separation in a diblock copolymer thin film. This flat film then serves as a highly ordered chemical template for metal nanostructure growth in a variety of pattern morphologies [5]. The large-area periodically nanopatterned sample systems are especially very well suited for x-ray and neutron scattering experiments.

In this contribution, we outline the reverse epitaxy mechanism and present examples of how the resulting surface nanopatterns can be employed in the fabrication of nanostructure arrays. We hope to stimulate discussion of further applications by emphasizing the simplicity and versatility of this bottom-up approach.

[1] H.A. Atwater and A. Polman, Nature Materials 9 (2010)
[2] J. Vogt et al., Phys. Chem. Chem. Phys. 17 (2015)
[3] D. Grundler, Nature Physics 11 (2015)
[4] X. Ou et al., Nanoscale 7 (2015)
[5] D. Erb et al., Science Advances 1 (2015)

Primary authors:
ERB, Denise (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany))

Co-authors :
OU, Xin (Chinese Academy of Sciences, Shanghai Institute of Microsystem and Information Technology, Shanghai (China)) SCHLAGE, Kai (Deutsches Elektronen-Synchrotron, Photon Science Division, Hamburg (Germany)) LENZ, Kilian (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany)) RöHLSBERGER, Ralf (Deutsches Elektronen-Synchrotron, Photon Science Division, Hamburg (Germany)) LINDNER, Jürgen (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany)) FACSKO, Stefan (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany)) HELM, Manfred (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany)) FASSBENDER, Jürgen (Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden (Germany))

Silicon Nanowires with NiSi2 Contacts – Towards Reconfigurable Devices

Content:

Reconfigurable transistors (RFETs) can be switched between electron and hole current by changing the polarity of the gate potential. This allows a much higher functionality and hence, logic operations can be realized with fewer transistors. In our research we investigate RFETs by simulations and by fabricating devices experimentally.

Devices are built using a top-down approach by electron beam lithography and reactive ion etching. The process is highly optimized to build well defined nanowires with variable diameters. Contacts are created by nickel silicidation. Electrical measurements are performed and compared for two different crystal orientations of the SiNWs. It is demonstrated that electron and hole current is more symmetric in case of <100> SiNWs in contrast to <110> SiNWs, which is advantageous for building RFETs.

Since the functionality of RFETs is mainly determined by the interface, quantum transport simulations are performed to calculate the transmission function through a NiSi2-Si interface. Transfer characteristics are then calculated based on a simplified model for a RFET. Based on this model, the impact of strain is investigated. It is found that compressive strain can result in symmetric electron and hole currents, which is in reasonable agreement with existing literature data.

Primary authors:
Mr. FUCHS, Florian (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany)

Co-authors :
Mr. DEB, Dipjyoti (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany) Mr. KHAN, Muhammad Bilal (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany) Prof. GEMMING, Sibylle (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany) Dr. SCHUSTER, Jörg (Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany) Dr. ERBE, Artur (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany)

Single bunch extraction by SAW driven bunch chopper

Content:

Surface acoustic waves (SAWs) travel on the surface of solids, temporarily creating grating-like structures with amplitude up to one nanometer and near-sinusoidal deformation profile. Using this effect Tucoulou et al. demonstrated the feasibility of a high frequency chopper for synchrotron radiation at ESRF [1]. But due to the fact that the velocities of the SAW are typically on the order of 3000m/s, the time resolution of the device was limited by the value of ~1 ms due to the large travel distance of the SAW pulse through the footprint of x-ray beam at a small grazing incidence angle. To overcome this problem we performed the measurements in Bragg sagittal diffraction geometry [2]. In sagittal diffraction the SAW grating grooves are parallel to the direction of the incoming beam, and due to the shorter propagation length needed for effective X-ray diffraction on SAWs this geometry is much more promising. The Bragg reflection on a Si/W multilayer was used. SAW with frequencies up to 500 MHz was excited in piezoelectric materials using interdigital transducer (IDT) deposited on the surface. The experiment was performed by electronic pulsing of the SAW emission and synchronization with the arrival of the synchrotron X-ray pulses. The achieved time resolution was in the order of 100 ns.

[1] R. Tucoulou et al., Nuclear Instruments and Methods in Physics Research B 132, 207-213 (1997)
[2] D.V. Roshchupkin et al., Journal of Applied Physics, 110 (2011)

Primary authors:
Mr. VADILONGA, Simone (Helmholt Zentrum berlin)

Co-authors :
Dr. ZIZAK, Ivo (Helmholt Zentrum berlin) Mr. PETSIUK, Andrei (Helmholt Zentrum berlin) Prof. ERKO, Alexei (Helmholt Zentrum berlin) Dr. ROSHCHUPKIN, Dmitri (IMT RAS)

Slow internal protein dynamics in solution observed by Neutron Spinecho Spectroscopy

Content:

The biological function of proteins is often related to large-scale domain motions, which are sometimes induced or suppressed by the binding of a substrate or due to cosolvents. Configurational changes are often observed by methods like x-ray crystallography giving a static image of the protein structure and suppressing large-scale domain motions, which occur in solution. Observed configurational changes can be related to the substrate binding or the crystal packing, which favors specific configurations. On the other side domain motions can be related to soft hinges, flexible linker regions or -as in the case of natively unfolded proteins- be intrinsic to the unfolded structure if the protein is unrestricted in solution. These large-scale domain motions in solution cannot be observed by X-ray crystallography or NMR spectroscopy. Small angle scattering by X-rays or neutrons in combination with neutron spin echo spectroscopy (NSE) can be used to observe configurational changes and equilibrium dynamics between functional domains on several nanoseconds.
I present here examples of large-scale structure determination by SANS and SAX combined with NSE to determine the dynamics of the proteins on nanometer length scale and a timescale up to hundred nanoseconds. Different types of motions related to the structure can be observed. Phosphoglycerate kinase shows a clear hinge motion [1] . Lactoferrin shows a dumbbell structure with □□helical soft linker [2]. By thermal unfolding of Ribonuclease A the transition of a rigid protein to an unfolded chain with 4 disulfide bonds can be observed showing the restriction of the disulfide bonds. Immunoglobulin 1 (IGG1) presents a strong dynamics due to the short linkers connecting the Fc with the Fab fragment [3]. Analysis by a Ornstein-Uhlenbeck process result in the determination of friction and spring constants.
Overall neutron scattering is shown to be a unique tool to examine the micromechanics of proteins on the length scale of domains with the ability to examine forces and friction.

References
(1) Inoue, R.; Biehl, R.; Rosenkranz, T.; Fitter, J.; Monkenbusch, M.; Radulescu, A.; Farago, B.; Richter, D. Biophys J 2010, 99 (7), 2309.
(2) Sill, C.; Biehl, R.; Hoffmann, B.; Radulescu, A.; Appavou, M.-S.; Farago, B.; Merkel, R.; Richter, D. BMC Biophys. 2016, 9 (1), 7.
(3) Stingaciu, L. R.; Ivanova, O.; Ohl, M.; Biehl, R.; Richter, D. Sci. Rep. 2016, 6, 22148.

Primary authors:
Dr. BIEHL, Ralf (Forschungszentrum Jülich JCNS-1)

Soft x-ray spectroscopy on Photosystem II and prototypical metal complexes

Content:

3d transition metals play a crucial role as reaction centers for catalysis in a variety of metalloproteins. With the advances of high-brilliance x-ray free-electron lasers (XFELs) x-ray spectroscopic studies on dilute metalloproteins with (sub)millimolar concentrations becomes increasingly accessible, unravelling the local electronic structure and potentially the biologic function.
A key example is the Photosystem II protein (PS II), which upon visible light absorption in a four-electron redox reaction oxidizes water molecules at its Mn4CaO5 catalytic site. Experimentally mapping and understanding this reaction on a molecular and electronic level may provide chances for the development of efficient biomimetic systems.
We present seminal results on soft x-ray absorption spectroscopy (XAS) on Photosystem II at the Mn L-edge in order to track local electronic and structural changes in the Mn4CaO5 cluster of PS II in the time course of the water oxidation reaction. We combine an in-vacuum liquid sample delivery with a high-efficiency zone-plate spectrometer for measuring partial fluorescence yield XAS on the Mn L-edge of PS II solution sample under physiological conditions. In a “probe-before-destroy”-approach femtosecond soft x-ray pulses delivered by the soft x-ray beamline at the XFEL Linac Coherent Light Source (LCLS) probe the sample before the onset of x-ray induced sample damage.
Here we present and discuss our recent progress on Mn L-edge XAS on PS II and compare the results to those obtained from structural mimics of the Mn4CaO5 cluster, measured under similar conditions. An outline to the interpretation of the spectra in an ab-initio theoretical framework is discussed on the basis of complementary PFY-XAS spectra of mononuclear Mn-complexes.

Primary authors:
Mr. KUBIN, Markus (Helmholtz-Zentrum Berlin, Germany)

Co-authors :
KERN, Jan (Lawrence Berkeley National Laboratory, USA) CHATTERJEE, Ruchira (Lawrence Berkeley National Laboratory, USA) GUL, Sheraz (Lawrence Berkeley National Laboratory, USA) FULLER, Franklin (Lawrence Berkeley National Laboratory, USA) KROLL, Thomas (Stanford Linear Accelerator Laboratory, USA) GUO, Meiyuan (Uppsala University, Sweden) LUNDBERG, Marcus (Uppsala University, Sweden) ODELIUS, Michael (Stockholm University, Sweden) LöCHEL, Heike (Helmholtz-Zentrum Berlin, Germany) QUEVEDO, Wilson (Helmholtz-Zentrum Berlin, Germany) ERKO, Alexei (Helmholtz-Zentrum Berlin, Germany) FöHLISCH, Alexander (Helmholtz-Zentrum Berlin, Germany) BERGMANN, Uwe (Stanford Linear Accelerator Laboratory, USA) MITZNER, Rolf (Helmholtz-Zentrum Berlin, Germany) YACHANDRA, Vittal (Lawrence Berkeley National Laboratory, USA) YANO, Junko (Lawrence Berkeley National Laboratory, USA) WERNET, Philippe (Helmholtz-Zentrum Berlin, Germany)

Spin structure in the ferroelectric phase of multiferroic Y-type hexaferrite Ba(2-x)SrxZn2Fe12O22

Content:

Magnetoelectric hexaferrites have widened the bottleneck for practical applications in memory devices or MFRAM by bringing the operating temperature close to room temperature. Above room temperature magnetic ordering temperature in hexaferrite due to strong Fe-O-Fe superexchange interaction makes them a potential candidate from application point of view. Room temperature magnetoelectric coupling has been realized in a relatively complex z-type hexaferrite. Y-type hexaferrite Ba(2-x)SrxZn2Fe12O22 is one of the prototypes of the hexaferrite family where H-induced ferroelectric polarization was found. The spin structure found till now in ferroelectric phase is a 2-fan planar structure, which is inconsistent with inverse Dzyaloshinskii-Moriya (IDM) or spin current mechanism. We used soft-x-ray resonance and neutron scattering experiments to investigate the spin structure at different H and T (temperatures). In our in-field soft-x-ray resonance diffraction we found circular dichroism in horizontal field and linear dichroism in vertical field in the only observed commensurate (0 0 3/2) satellite reflection in the ferroelectric phase. This eventually established the spin structure to be transverse conical instead of a planar 2-fan. Our transverse conical structure is found to be present in as low field as 0.1 T at low temperatures and at room temperature (RT) also. This opens up a possibility of macroscopically observing H-induced polarization at low H and RT. We carried out the mapping of spin chiral domains at different H and T under diffraction conditions. Our observations of inversion of spin chiral domain configuration upon reversing the direction of H indicates that vector chirality switches direction upon reversing the direction of H. This eventually leads to polarization flipping with flipping magnetic fields, however macroscopically electric polarization was found to retain direction upon reversing H-direction, which can be attributed to difference in composition. in Field neutron scattering experiments also confirmed the spin structure with a c-component of magnetic moment in the ferroelectric phase. In addition we observed a canted ferrimagnetic phase above the ferroelectric phase, providing vital information that up to high field (6 T) c-component of the moment from the transverse cone is retained.

References

[1] T. Kimura et al., Phys. Rev. Lett. 94, 137201 (2005).
[2] N. Momozawa et al., JPSJ. 62, 1292 (1993).
[3] A. Mulders et al., Phys. Rev. B. 81, 092405 (2010).
[4] E. Schierle et al., Phys. Rev. Lett. 105, 167207 (2010).
[5] A. J. Hearmon et al., Phys. Rev. B. 84, 064418 (2011).

Primary authors:

Mr. THAKURIA, Pankaj (Peter Gr¨unberg Institut PGI and J¨ulich Center for Neutron Science JCNS, JARA-FIT, Forschungszentrum J¨ulich GmbH, 52425 J¨ulich, Germany)

Co-authors :

Mr. KHAZARADZE, Giorgi (Peter Gr¨unberg Institut PGI and J¨ulich Center for Neutron Science JCNS, JARA-FIT, Forschungszentrum J¨ulich GmbH, 52425 J¨ulich, Germany) Dr. SCHIERLE, Enrico (Helmholtz-Zentrum Berlin f¨ur Materialien und Energie, Wilhelm-Conrad-R¨ontgen-Campus BESSY II, Berlin, Germany) Dr. PROKE˘S, Karel (Helmholtz-Zentrum f¨ur Materialien und Energie, BER-II, Germany) Prof. ANGST, Manuel (Peter Gr¨unberg Institut PGI and J¨ulich Center for Neutron Science JCNS, JARA-FIT, Forschungszentrum J¨ulich GmbH, 52425 J¨ulich, Germany)

Spin-lattice effects in high magnetic fields

Content:

Spin-lattice effects play an important role in many frustrated magnets. In this work, we show some examples of such effects observed in the quantum spin-ice candidates, Yb2Ti2O7 [1] and Tb2Ti2O7, and the strongly frustrated antiferromagnet CdCr2O4 [2]. A combination of ultrasound technique with low temperatures and high magnetic fields provides valuable information about the spin-lattice interactions. Specifically, phase transitions and critical phenomena in various magnetic systems can be successfully investigated by means of the sound velocity and sound attenuation measurements.

[1] Subhro Bhattacharjee, S. Erfanifam, E.L. Green, M. Naumann, Zhaosheng Wang, S. Granovski, M. Doerr, J. Wosnitza, A.A. Zvyagin, R. Moessner, A. Maljuk, S. Wurmehl, B. Büchner, and S. Zherlitsyn, Phys. Rev. B 93, 144412 (2016).
[2] S. Zherlitsyn, V. Tsurkan, A.A. Zvyagin, S. Yasin, S. Erfanifam, R. Beyer, M. Naumann, E. Green, J. Wosnitza, and A. Loidl, Phys. Rev. B 91, 060406(R) (2015).

Primary authors:
ZHERLITSYN, S. (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany)

Co-authors :
GRITSENKO, Y. (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany) WOSNITZA, J. (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany) TSURKAN, V. (Universität Augsburg, 86159 Augsburg, Germany) LOIDL, A. (Universität Augsburg, 86159 Augsburg, Germany) MOESSNER, R. (Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany) WURMEHL, S. (Leibniz-Institut für Festkörper- und Werkstoffforschung, 01069 Dresden, Germany) BüCHNER, B. (Leibniz-Institut für Festkörper- und Werkstoffforschung, 01069 Dresden, Germany) GREEN, E.l. (Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany) FENNELL, T. (Paul Scherrer Institut, 5232 Villigen PSI, Switzerland) KENZELMANN, M. (Paul Scherrer Institut, 5232 Villigen PSI, Switzerland)

Spin-wave and Electromagnon Dispersions in Multiferroic MnWO4 as Observed by Neutron Spectroscopy

Content:

So-called spin-driven ferroelectrics, for which the inversion symmetry is broken in the ferroelectric phase due to the appearance of a particular magnetically ordered state, provide a path to the required coupling1,2. As a prototypical multiferroic material with spiral magnetic order, MnWO4 has been widely studied concerning its magnetic and ferroelectric properties3,4. However, a deeper insight into the coupling between the electric and magnetic degrees of freedom can be gained by studying not only the respective order but also the excitation spectra. In present work, high resolution inelastic neutron scattering reveals that the elementary magnetic excitations in multiferroic MnWO4 consist of low energy dispersive electromagnons in addition to the well-known spin-wave excitations5. The latter can well be modeled by a Heisenberg Hamiltonian with magnetic exchange coupling extending to the 12th nearest neighbor. They exhibit a spin wave gap of 0.61(1) meV. Two electromagnon branches appear at lower energies of 0.07(1) meV and 0.45(1) meV at the zone center. They reflect the dynamic magnetoelectric coupling and persist in both, the collinear magnetic and paraelectric AF1 phase, and the spin spiral ferroelectric AF2 phase. These excitations are associated with the Dzyaloshinskii-Moriya exchange interaction, which is significant due to the rather large spin-orbit coupling.

References:
[1] S.-W. Cheong and M. Mostovoy, Nature Mater. 6, 13(2007).
[2] Y. Tokura, S. Seki and N. Nagaosa, Rep. Prog. Phys. 77, 076501(2014).
[3] O. Heyer et al., J. Phys.: Condens. Matter 18, L471(2006).
[4] K. Taniguchi et al., Phys. Rev. Lett. 97, 097203(2006).
[5] Y. Xiao et al., Phys. Rev. B 93, 214428(2016).

Primary authors:
XIAO, Y. (Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany)

Structural organization of the ultra-hard magnetic biominerals in chiton radula teeth

Content:

Nature provides many archetypes of highly ordered systems, some of these biomaterials are known for their remarkable mechanical properties. An amazing example of biomaterials is the tooth of chitons. The fully mineralized chiton tooth displays remarkable functional properties such as outstanding fracture toughness, wear resistance and has the highest reported hardness among known biominerals. The excellence functional properties of the resulting mineral composites can be attributed to the buried organic–inorganic interfaces at multiple hierarchical levels and the highly mineralized inorganic content (ca. 70 wt. %). They are hardened by the inclusion of magnetite nanoparticles (15-50 nm) into a protein-polysaccharide fibrous matrix. The magnetite nanocrystals are aligned parallel to the cusp’s surface along its contours. The arrangement and orientation of this ultrastructure plays an important role for the mechanical properties of inhomogeneous and anisotropic materials.
In the present work we have done several characterization experiments on the chiton teeth by using SEM, TEM, SANS and SAXS/WAXS. By such methods, nanoscale structure changing over macroscopic length scales is pivotal to understanding the function of hierarchically organized tissues and materials. They are allowed to spatially resolve and quantify the material's ultrastructure orientation in a nanoscale context. From the investigation, it is clear that the tooth show a typical core-shell structure. The shell is composed of magnetic magnetite nanocrystals embedded into a protein-polysaccharide fibrous matrix, while the core is composed of apatite. Results show that clearly mineral phase and orientation changes in the teeth core region and teeth shell region. Further, we explore the magnetite mineralization kinetics by using micro focus SAXS/WAXS which can be found in teeth with different mineralized state. We aimed to provide a novel insight establishing a direct relation between the hierarchical structure and the mineralized particles/organic matrix producing such highly and optimized sophisticated materials properties. These structural and mineralization mechanism are compared with the synthetic samples. The comparative studies of the structural features will help to optimize the materials structure for improved mechanical performance.

Primary authors:
Dr. WU, Baohu (JCNS, Forschungszentrum Jülich)

Co-authors :
Mr. DEBUS, Christian (Physical Chemistry, Uni-Konstanz) Dr. FAIVRE, Damien (MPI Colloids & Interfaces, Potsdam) Dr. DIETMAR, Schwahn (FRMII, TUM) Prof. CöLFEN, Helmut (Physical Chemistry, Uni-Konstanz) Dr. PIPICH, Vitaliy (JCNS MLZ, Forschungszentrum Jülich)

Structure and Dynamics of PEGylated proteins: Structure and dynamics of PEGylated phosphoglycerate kinase

Content:

PEGylation - the covalent attachment of polyethylene glycol e.g. via maleimide (mPEG) - of bioactive proteins is a widely used technique to improve delivery, biocompatibility and bioavailability of therapeutics and is used in commercial pharmaceutics as Certolizumab pegol and others[1]. The properties of PEG such as good water solubility, lack of toxicity and low immunogenicity can be extremely useful in drug design as it can increases drug solubility and stability, increases circulating time, reduce immune response or may increase biological activity. Many of PEGylated proetins have been approved for therapeutic use by the U.S. Food and Drug Administartion e.g. PEG L-asparaginase used to treat acute lymphocytic leukemia (ALL) in ERT (Enzyme replacement therapy) where the attachment of PEG to protein decrease the side effects which is due to administration of the enzymes. It seems that adding PEG to enzymes may dramatically change the possibility of using the PEGylated proteins in many medical applications. However the biological activity and structural changes of protein (especially enzymes used in ERT) due to PEG are not yet good examined. The structural and functional stability of protein seems to be unaffected by PEGylation as observed for BSA by standard biophysical methods [2,3]. The conformation of the PEG around the protein is still under debate. Le Cœur describes for hemoglobinthe conformation as a dumbbell structure below a molecular weight of 10kDa, while above a more compact structure is found (maybe wrapped at the surface) [3]. This effect may depend on the protein surface chemistry.
In our present study we focus on PGK and BSA (Bovine serum albumin) to observe the influence of PEGylation on structure and dynamics. Phosphoglycerate kinase (PGK) is an enzyme that catalyses the reversible transfer of a phosphate group from 1,3-bisphosphoglycerate (1,3-BPG) to ADP producing 3-phosphoglycerate (3-PG) and ATP (see figure 1). It has been known that ligand binding (ATP, 3-GP) causes a cleft closing of PGK [4]. We have shown by SANS that the cleft closing is not strong enough to allow activity [5]. By neutron spinecho spectroscopy (NSE) we have show that the thermal large-scale domain motions on a 40 ns timescale allows to reach the active configuration and enables activity [5]. We now use a PGK mutant, with one cysteine at Gln135 at the surface that allows attachment of a single mPEG chain to the protein. The attached mPEG may affect the internal functional dynamics of the PGK by a direct influence onto the protein structure or by modification of the local environment as e.g. the protein surface friction. We want to examine the influences of PEGylation onto conformational changes induced by the ligands and the influence on domain dynamics by combining SAXS, SANS and NSE. The conformational changes detected by SAXS and SANS (measured with D2O matched mPEG), enzymatic assay and NSE measurements of the protein dynamics may help us to understand the real influence of mPEG on structure and function of PGK. Additionally, the mPEG conformation around the protein influences the interactions between PEGylated proteins and can be measured by accessing the structure factor. This may help to understand how to increase the drug concentration in medical applications.
References
[1] Roberts, M. J.; Bentley, M. D.; Harris, J. M. Advanced Drug Delivery Reviews. 2012, pp 116–127.
[2] B. Plesner, C.J. Fee, P. Westh, A.D. Nielsen, Eur J Pharm Biopharm 79, 399-405 (2011)
[3] Le Cœur, et al.Langmuir 2015, 31 (30), 8402–8410.
[4]Varga A, Flachner B, Konarev P et al., FEBS Lett. 2006, 580(11), 2698-706.
[5] Inoue, R., R. Biehl, T. Rosenkranz, J. Fitter, M. Monkenbusch, A. Radulescu, B. Farago, D. Richter. 2010. Biophys J. 99: 2309–2317.

Primary authors:
Dr. CIEPLUCH, Karol (Forschungszentrum Jülich, Istitute of Complex Systems (ICS-1))

Co-authors :
Dr. BIEHL, Ralf (Forschungszentrum Jülich, Istitute of Complex Systems (ICS-1)) Prof. RICHTER, Dieter (Forschungszentrum Jülich, Istitute of Complex Systems (ICS-1))

Structure investigations of magneto-elastomeric nanocomposites

Content:

Superparamagnetic iron oxide nanoparticles (SPIONs) encapsulated with a diblock copolymer consisting of a polydiene and poly(ethylene oxide) (PEO) were synthesized and dispersed into a PEO matrix. Using different polydienes and variable crosslinking methods results in highly stable SPIONs which can be characterized by small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). These investigations show the presence of mostly single nanoparticles and a small amount of agglomerates of a few particles. Therefore, it is of great value to efficiently control the encapsulation and synthetic conditions regarding the minimization of agglomerates and creation of uniform hybrid nanomaterials.

Primary authors:
Mrs. FRUHNER, Lisa (Forschungszentrum Jülich) Dr. KRUTYEVA, Margarita (Forschungszentrum Jülich)

Co-authors :
Mr. FELD, Artur (University of Hamburg) Ms. KOLL, Rieke (University of Hamburg) Dr. PYCKHOUT-HINTZEN, Wim (Forschungszentrum Jülich) Dr. HELLER, Hauke (University of Hamburg) Dr. ALLGAIER, Jürgen (Forschungszentrum Jülich) Prof. WELLER, Horst (University of Hamburg)

Studies on Yb and Sm based pyrochlores

Content:

In this poster, we present our studies of powder samples of $Yb_2Ti_2O_7$, $Sm_2Ti_2O_7$ and $Sm_2Sn_2O_7$. Pyrochlores are subject to the formation of defective structures, which is known to highly influence the geometrical frustration mechanism at low temperatures [1,2]. We have proven the stoichiometry of our samples with neutron and x-rays diffraction and shown that they all present a low temperature specific heat anomaly, characteristic of pristine samples of $Yb_2Ti_2O_7$, but yet not shown in Sm based compounds. We report neutron diffraction data of $Yb_2Ti_2O_7$ that clearly display a phase transition to a long-range, ferromagnetic state at T_C=0.28 K, in disagreement with the recent works that state that the phase transition seen in neutron scattering is unrelated to that seen in heat capacity measurements [3,4]. The observed absence of the (200) magnetic Bragg peak in our work indicates that the canting angle of the spins out of the cubic axis is much smaller than previously reported [3], making the structure a quasi-collinear ferromagnet with an ordered moment of 0.87(2) μB. Additionally, we show that our Yb sample does not adopt any other symmetry-allowed long-range magnetic order below T_C and that in fact we observe no evidence of multiple phase transitions or a multi-step ordering process [5].

[1]Ross, K. A. et al. Physical Review B 84, 094437 (2011)
[2]Ross, K. A. et al. Physical Review B 84, 174424 (2012)
[3]Gaudet, J. et al. Physical Review B 93, 064406 (2016)
[4]Lhotel, E. et al. Physical Review B 89, 224419 (2014)
[5]Jaubert, L. D. C. et. al. Physical Review Letters 115, 267208 (2015)

E-mail of the corresponding author: v.pecanha.antonio@fz-juelich.de

Primary authors:
PECANHA-ANTONIO, Viviane (JCNS at MLZ, Forschungszentrum Jülich GmbH)

Co-authors :
FENG, Erxi (JCNS at MLZ, Forschungszentrum Jülich GmbH) SU, Yixi (JCNS at MLZ, Forschungszentrum Jülich GmbH) BRÜCKEL, Thomas (JCNS and PGI, Forschungszentrum Jülich GmbH)

Study of 3D strain and damage interactions in thin-sheet Al alloy materials by synchrotron laminography and digital volume correlation

Content:

To provide lighter and optimized thin-walled components and materials for transportation, knowledge about the characteristic ductile damage mechanisms of metal sheets during forming and in service is necessary.
We apply synchrotron laminography and digital volume correlation to investigate the strain and damage interactions during tearing of ductile Al alloy sheet materials. Laminography allows us to image regions of interest three-dimensionally in large flat specimens. Digital volume correlation is based on the tracking of 3D laminography image contrast, which is caused by µm-sized internal voids and inclusions. Simultaneous assessment of 3D strain and damage at a distance of 1 mm from a notch of a thin compact-tension-like specimen shows parallel crossing slant strained bands which are active from the beginning of loading in a region where the final crack will be slant. These bands have intermittent activity but are relatively stable in space. Materials with different work hardening properties are assessed and show very similar strain concentration patterns and final failure characteristics.

Primary authors:
Dr. HELFEN, Lukas (IPS, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany)

Co-authors :
Dr. MORGENEYER, Thilo F. (Centre des Matériaux, MINES Paristech, CNRS, UMR 7633, 10 rue Henri Desbruères BP 87, F-91003 Evry Cedex) Dr. CHENG, Yin (IPS, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany) BULJAC, Ante (LMT-Cachan, 61 avenue du President Wilson, F-94235 Cachan Cedex, France) Dr. HILD, Francois (LMT-Cachan, 61 avenue du President Wilson, F-94235 Cachan Cedex, France) Prof. BAUMBACH, Tilo (IPS, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany)

Study of Mn1.9Co0.1Sb

Content:

Reportedly, Co-modified Mn2Sb system exhibits three different magnetically ordered states, which makes it potentially interesting in terms of magnetocaloric effect. We report on preparation and characterization of powder as well as a single crystal of Mn1.9Co0.1Sb. We synthesize polycrystalline samples in a cold crucible using induction melting process. Then we check the quality of sample with x-ray powder diffraction and Laue camera for powder and single crystal respectively. We analyzed the x-ray data with the Le-bail method and observed the change in lattice parameter. Apart from that, to study macroscopic magnetic properties, we carried out magnetization measurements with vibration sample magnetometer. After having measured a sample along different crystallographic orientations, we were able to observe the magnetic anisotropy and some interesting implications in comparison to powder data.

Primary authors:
Mr. CHIKOVANI, Mamuka (Forschungszentrum Juelich GmbH)

Co-authors :
Dr. FRIESE, Karen (Forschungszentrum Juelich GmbH) Dr. VOIGT, Jorg (Forschungszentrum Juelich GmbH) PERSSON, Jorg (Forschungszentrum Juelich GmbH) Prof. BRUECKEL, Thomas (Forschungszentrum Juelich GmbH)

Study of influence of the applied voltage bias on the strain field in a single GaN nanowire

Content:

In the poster, the results of our recent beamtime at PETRA III will be presented. In the experiment, we applied the coherent x-ray diffraction technique to study the strain field of a single GaN nanowire (NW) with nanometer-scale spatial resolution under applied voltage bias along the growth [0001] direction of the NW. From the series of measurements performed at different voltage values and polarities, we reveal the 3D strain field evolution of the NW while varying the external electric field.

Primary authors:
Dr. LAZAREV, Sergey (DESY)

Co-authors :
DZHIGAEV, Dmitry (DESY) Dr. ZOZULYA, Alexey (DESY) ZALUZHNYY, Ivan (DESY) GOROBTSOV, Oleg (DESY) Dr. SPRUNG, Michael (DESY) Prof. VARTANIANTS, Ivan (DESY)

Studying thin-film solar cells and battery materials using electron and soft x-ray spectroscopy

Content:

In this talk, we will present our recent progress on studying thin-film solar cells and battery materials using electron and (in-situ) soft x-ray spectroscopy. Such devices typically consist of a multilayer structure, with each layer addressing a specific function (e.g., light absorption, electrical contact formation, band alignment engineering). For further optimization of the devices, a detailed knowledge of the electronic and chemical properties at the interfaces between these layers is crucial. Using selected examples, this presentation will show the power of electron and soft x-ray spectroscopies, namely photoelectron spectroscopy, inverse photoemission, (soft) x-ray absorption spectroscopy, x-ray emission spectroscopy, and resonant inelastic x-ray scattering, for studying such applied systems. Particular focus is placed on studying samples which are as close as possible to the relevant device production process while still fulfilling the requirements of the specific experimental technique. It is found that the combination of the named techniques is particularly powerful when employing their complementary information content and wide range of information depths.

Primary authors:
Dr. WEINHARDT, Lothar (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT))

Co-authors :
Dr. HAUSCHILD, Dirk (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Dr. KREIKEMEYER-LORENZO, Dagmar (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Mrs. WACHS, Susanne (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Dr. LEON, Aline (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT)) Prof. HESKE, Clemens (Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT))

Surface structure of Fe3O4 under varying conditions studied by surface x-ray diffraction

Content:

Magnetite (Fe3O4) exhibits interesting properties which makes it attractive for applications in catalysis and spintronic devices. Since these applications depend on the surface properties of magnetite, it is important to understand its surface structure under different conditions. The (001) surface of magnetite shows a (√2×√2)R45° surface reconstruction in UHV which gets lifted upon water adsorption at room temperature. Although previous experiments on the (001) surface identified a possible surface structure, recent observations led to a new model.
To clarify this controversy and to get insight into changes in the surface structure at varying conditions, we studied the surface structure of a natural Fe3O4 (001) single-crystal by surface x-ray diffraction in ultra-high vacuum at the ID03 beamline at the ESRF at 11 keV photon energy as well as at the Sixs beamline at Soleil at 12 keV. We repeated the same measurements while exposing the surface to water vapor. Our data shows a much better level of agreement with the new model than with the old one. Upon dosing water vapor, the reconstruction gets lifted irreversible. Finally we went to water-gas shift reaction conditions by flowing water and CO simultaneously over the surface at different temperatures, observing a strong roughening in the process as well as changes in the correlation length of the surface structure.

Primary authors:
Mr. ARNDT, Björn (Desy, University of Hamburg)

Co-authors :
Dr. NOEI, Heshmat (Desy) Dr. GRAANAES, Elin (Desy) Mr. CREUTZBURG, Marcus (Desy, University of Hamburg) Mr. VOLKOV, Sergey (Desy) Mr. BLIEM, Roland (Vienna University of Technology) Mr. GAMBA, Oscar (Vienna University of Technology) Mr. PARKINSON, Gareth (Vienna University of Technology) Prof. DIEBOLD, Ulrike (Vienna University of Technology) Prof. STIERLE, Andreas (Desy, University of Hamburg)

THz-based FELs and attosecond sources

Content:

Recent years have witnessed extensive efforts pursuing realization of compact X-ray sources. Almost all the various proposed scenarios are inspired by the free electron laser (FEL) concept, where relativistic electrons exiting linear accelerators are forced to wiggle and consequently radiate. In a conventional FEL, RF accelerators operate in conjunction with magnetic undulators leading to the today large X-ray facilities. The dominant factor determining the cost and size of electron accelerators is the achievable accelerating gradient. Conventional high-brightness radio-frequency accelerating structures operate with 30–50 MeV/m gradients. Electron accelerators driven with optical or infrared sources have demonstrated accelerating gradients orders of magnitude above that achievable with conventional radio-frequency structures. However, laser-driven wakefield accelerators require intense femtosecond sources and direct laser-driven accelerators suffer from low bunch charge, sub-micron tolerances and sub-femtosecond timing requirements due to the short wavelength of operation. This contribution presents the novel use of recently available high power THz sources and optical lasers to realize compact FEL setups in the AXSIS project at CFEL in Hamburg, funded by the European Research Council. The scheme starts with injecting and accelerating electrons using intense THz fields, where high-gradient fields produce relativistic electrons in millimeter size structures. Subsequently, the generated electrons collide with a counter-propagating optical laser, which causes a wiggling motion with micro-meter size period. Ultimately, X-ray pulses with angstrom-level wavelengths will be radiated out of the wiggling electrons. The accomplished theoretical studies as well as experimental demonstrations towards realizing a THz-FEL will be outlined and explained.

Primary authors:
Dr. FALLAHI, Arya (CFEL)

Tailored thermal conductivity in thin film multilayers

Content:

Thermal conductivity in thin films plays an important role in functional materials for information technology or energy harvesting (thermoelectrics) [1]. Conductivity can be tailored beyond pure material properties by introducing interfaces, in particular in multilayered nanoscaled systems.
We study the effect on these boundaries on phonon transport to elucidate the mechanisms that govern the changes in thermal conductivities. Two systems are compared, which represent extremes for phonon interactions: (i) a silicon-based multilayer assembly, where the individual sublayers are composed of alternating silicon isotopes. Thus, electronic transport is not affected, only phonon modes are influenced. The unexpected strong reduction in thermal conductivity is discussed in terms of coherent transport, in particular Umklapp scattering [2-5]. (ii) High-impedance mismatch layers composed of Si/Mo multilayers are discussed, which possess an extremely low thermal conductivity. The connection to stacking and structure of the layers is discussed.

We would like to acknowledge beamtime at ESRF and ANKA and support by M. Wulff, D. Khakhulin, N. Smale, E. Huttel and N. Hiller. This work is supported within priority program 1386 and the Heisenberg fellowship of the DFG.

[1] Snyder G J and Toberer E S, Nature Mater. 2008, 7, 105.
[2] Bracht H, Wehmeier N, Eon S, Plech A, Issenmann D, Lundsgaard Hansen J, Nylandsted Larsen A,
Haller E E and Ager III J W, Appl. Phys. Lett. 2012, 101, 064103.
[3] Bracht H, Eon S, Frieling R, Plech A, Issenmann D, Wolf D, Lundsgaard Hansen J, Nylandsted Larsen A, Ager III J W, Haller E. E., New. J. Phys. 2014, 16, 015021
[4] Issenmann D, Eon S, Bracht H, Hettich M, Dekorsy T, Buth G, Steininger R, Baumbach T, Lundsgaard Hansen J, Nylandsted Larsen A, Ager III J W, Haller E E, Plech A, phys. stat. sol. (a) 2016, 213, 541.
[5] Eon S, Frieling R, Plech A, Bracht H, phys. stat. sol. (a) 2016, DOI: 10.1002/pssa.201532607

Primary authors:
Dr. PLECH, Anton (Karlsruhe Institute of Technology)

Co-authors :
Prof. BRACHT, Hartmut (Institute for Materials Physics, U. Münster - Münster(Germany)) Mrs. EON, Soizic (Institute for Materials Physics, U. Münster - Münster(Germany)) Dr. FRIELING, Rafael (Institute for Materials Physics, U. Münster - Münster(Germany)) Dr. ISENMANN, Daniel (Karlsruhe Institute of Technology) Dr. KRAUSE, Bärbel (Karlsruhe Institute of Technology) Dr. BUTH, Gernot (Karlsruhe Institute of Technology) Dr. STEININGER, Ralf (Karlsruhe Institute of Technology) Prof. BAUMBACH, Tilo (Karlsruhe Institute of Technology)

Terahertz Radiation Driven Dynamics of Magnetic Domain Structures Probed by Free-Electron Laser Light

Content:

Controlling magnetism on ultra-fast time scales and on nanometer length scales is a challenge for modern research in magnetism. Means for inducing dynamics on these time scales are femtosecond optical lasers and THz sources. Probing the dynamics on a nanometer length scale is possible with free-electron laser sources.
We report on a THz-pump–XUV-probe scattering experiment on (Co/Pt)n multilayers (n = 8,16) with perpendicular magnetic anisotropy (PMA) exhibiting a maze domain pattern. An additional electromagnetic undulator available at FLASH was used to produce 10-cycle linearly polarized THz pulses. The fundamental wavelength was set to 150 µm and higher harmonics down to 30 µm have been used as a pump. The resulting dynamics have been probed on femtosecond time scales by resonant magnetic small-angle scattering at the cobalt M3 edge.
For a multilayer with 8-fold repetition we observed that after 200 fs the scattering intensity is drastically decreased by one order of magnitude. This change is fast compared to the duration of the THz pump pulse, which is about 6 ps long. Besides, a shift of the scattering peak position to lower Q-values by occurred. The latter is similar to what was found when using NIR pumping [4]. However, here we observed an onset of the peak shift delayed by about 100 fs with respect to the reduction in scattering intensity and a different shape of both signals. Such subtle differences were impossible to resolve in the previous experiments using NIR-pump pulses due to the larger temporal jitter (> 100fs). Interestingly, the response is found to be much weaker (scattering intensity) or not resolvable (peak shift) in case of a Co/Pt multilayer with 16-fold repetition. The major difference is the PMA of both samples. While the 16-fold multilayer has a strong PMA (K1,eff = 200kJ/m3) the 8-fold multilayer has an almost vanishing PMA (K1,eff = 30kJ/m3), so that it is much more susceptible to magnetic fields and hence the THz magnetic field can cause a significant tilting of the magnetization.

Primary authors:
Dr. MUELLER, Leonard (DESY FS-CXS) Prof. GRUEBEL, Gerhard (DESY FS-CXS) Prof. OEPEN, Hans Peter (Universitaet Hamburg) Dr. STOJANOVIC, Nikola (Desy FS-FL)

Co-authors :
Dr. BERNTSEN, Magnus Hardenson (KTH) Mr. SCHLEITZER, Stefan (DESY FS-CXS) Dr. ROSEKER, Wojciech (DESY FS-CXS) Dr. LEHMKUEHLER, Felix (DESY FS-CXS) Mr. RYSOV, Rustam (DESY FS-CXS) Mr. GOLZ, Torsten (Desy FS-FL) Dr. KOBS, Andre (DESY FS-CXS) Mr. BAGSCHIK, Kai (Universitaet Hamburg) Mr. WAGNER, Jochen (Universitaet Hamburg) Dr. FROEMTER, Robert (Universitaet Hamburg) Prof. GUTT, Christian (Universitaet Siegen)

The High Brilliance Neutron Source Project

Content:

In the near future many research reactors in Europe used for neutron experiments will be shut down. The European Spallation Source (ESS), although very powerful, cannot fill this gap alone. Compact accelerator driven neutron sources (CANS), like the proposed High Brilliance Neutron Source (HBS) [1] have the capability to fill the vacancies in the segment of low and medium flux neutron sources. For such a facility, the whole accelerator system, target and moderator concepts, beam extraction, guide systems, and the instruments have to be optimized in order to be competitive with modern research reactors. In this regard, the low primary particle energy in the MeV range has many advantages like: a small shielding volume; a guide system starting close to the target having a large acceptance angle; a small target/moderator volume resulting in a compact neutron field increasing the brightness; a smaller accelerator compared to spallation based neutron sources reducing the cost. A brief outline of the current project status will be presented with the achievements already reached and plans for the future.

[1] U. Rücker, et. al.; The Jülich high-brilliance neutron source project; The European Physical Journal Plus (2016), 131

Primary authors:
Dr. ZAKALEK, Paul (JCNS-2, Forschungszentrum Jülich GmbH)

Co-authors :
Mr. CRONERT, Tobias (JCNS-2, Forschungszentrum Jülich GmbH) Dr. RüCKER, Ulrich (JCNS-2, Forschungszentrum Jülich GmbH) Dr. BAGGEMANN, Johannes (JCNS-2, Forschungszentrum Jülich GmbH) Mr. DOEGE, Paul-emmanuel (JCNS-2, Forschungszentrum Jülich GmbH) Dr. GUTBERLET, Thomas (JCNS-2, Forschungszentrum Jülich GmbH) Prof. BRüCKEL, Thomas (JCNS-2, Forschungszentrum Jülich GmbH)

The quantum vacuum as a dispersive, nonlinear optical material

Content:

In contrast to the classical picture of the vacuum, the quantum vacuum consists of a sea of virtual particles, many of which are charged. Charged virtual pairs form vacuum dipoles, screening the electron charge and giving rise to its physical value. The application of a strong electromagnetic field necessarily affects the quantum vacuum giving rise to vacuum birefringence, resonant transitions and spontaneous pair production. In this sense, the quantum vacuum is best understood as a dispersive material which can be polarised and which can resonate. The possibility of detecting predicted vacuum resonances with today's technology is investigated. The theoretical and experimental steps necessary are detailed, and the possible insights for our understanding of the vacuum are discussed.

Primary authors:
Dr. HARTIN, Anthony (Uni-HH)

The twofold nature of Coulomb scattering in graphene

Content:

The ultrafast dynamics in graphene, which is of great interest from both a fundamental as well as an application oriented point of view, has been studied intensively during the last years and ascinating effects such as carrier multiplication have been found. Here we focus on the Coulomb scattering dynamics in the energetic vicinity of the Dirac point. Utilizing an optical anisotropy, we reveal the twofold nature of Coulomb scattering in graphene by polarization resolved pump-probe experiments. Coulomb scattering is the main mechanism that transforms an optical excited non-equilibrium carrier distribution into a thermalized one and dominates the initial carrier dynamics. Many publications report extremely fast Coulomb scattering rates and thermalization times in the order of tens of fs often only estimated because of limited time resolution in experiments. This is comprehensible as the linear band structure of graphene allows carriers to scatter along a line easily since this inherently fulfils energy and momentum conservation. However, in case of excitation with linearly polarized light, the initial carrier distribution is anisotropic in k space. This means thermalization needs also a redistribution in momentum direction additionally to the equilibration in energy. When scattering with optical phonons is suppressed by photo excitation at low energy, noncollinear Coulomb scattering is limiting the thermalization time to surprisingly long times (several ps) [1]. This contrasting behaviour, namely a fast equilibration in energy but a slow one in momentum space, is what we refer to as the twofold nature of Coulomb scattering in graphene.

[1] J. C. König-Otto, M. Mittendorff, T. Winzer, F. Kadi, E. Malic, A. Knorr, C. Berger, W. A. de Heer, A. Pashkin, H. Schneider, M. Helm, and S. Winnerl, Phys. Rev. Lett. 117, 087401 (2016).

Primary authors:
Mr. KöNIG-OTTO, Jacob C. (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Dr. MARTIN, Mittendorff (University of Maryland) Dr. WINZER, Torben (Technische Universität Berlin) Dr. KADI, Faris (Technische Universität Berlin) Prof. MALIC, Ermin (Chalmers University of Technology) Prof. KNORR, Andreas (Technische Universität Berlin) Dr. BERGER, Claire (Georgia Institute of Technology) Prof. DE HEER, Walt A. (Georgia Institute of Technology) Dr. PASHKIN, Alexej (Helmholtz-Zentrum Dresden-Rossendorf) Dr. SCHNEIDER, Harald (Helmholtz-Zentrum Dresden-Rossendorf) Prof. HELM, Manfred (Helmholtz-Zentrum Dresden-Rossendorf) Dr. WINNERL, Stephan (Helmholtz-Zentrum Dresden-Rossendorf)

Thermal and thermoelectric high-magnetic-field study of the multiband superconductor FeSe

Content:

We explored the high-magnetic-field behavior of the thermoelectric and thermal-transport coefficients to probe the quasiparticle excitations in the normal and superconducting phase of the multiband material FeSe. The small and compensated thermoelectric coefficients increase with decreasing temperature due to the temperature-dependent increase of the charge-carrier mobility and the dominant role of the small hole Fermi-surface pocket with remarkably low Fermi temperature. The measured longitudinal and transverse thermal conductivities imply that a highly anisotropic small superconducting gap forms at the electron pocket whereas an isotropic and larger gap forms at the hole pocket. Below 1 K, both thermal conductivities exhibit anomalies at the upper critical field, Hc2, and at a constant field H* around 14 T. These results support the existence of a distinct field-induced superconducting phase above H* which emerges with a presumed large spin-imbalance of the hole Fermi-surface pocket.

Primary authors:
Dr. ARSENIJEVIC, Stevan (Hochfeld-Magnetlabor Dresden HLD-EMFL, HZDR)

Co-authors :
Mr. WATASHIGE, Tatsuya (Kyoto University, Japan) Mr. YAMASHITA, Takuya (Kyoto University, Japan) Mr. TERAZAWA, Daiki (Kyoto University, Japan) Mr. ONISHI, Takafumi (Kyoto University, Japan) Mr. OPHERDEN, Lars (Hochfeld-Magnetlabor Dresden HLD-EMFL, HZDR) Prof. KASAHARA, Shigeru (Kyoto University, Japan) Dr. TOKIWA, Yoshifumi (Kyoto University, Japan) Prof. KASAHARA, Yuichi (Kyoto University, Japan) Prof. SHIBAUCHI, Takasada (University of Tokyo, Japan) Prof. VON LöHNEYSEN, Hilbert (Karlsruhe Institut für Technologie, Germany) Prof. WOSNITZA, Jochen (Hochfeld-Magnetlabor Dresden HLD-EMFL, HZDR) Prof. MATSUDA, Yuji (Kyoto University, Japan)

Thermalization of X-ray-generated electron cascades in diamond and LiF

Content:

Irradiation with low-fluence X-ray pulses leaves the target structurally undamaged; however, the radiation still excites hot electrons within the material. Here we discuss the kinetics of the laser-excited electrons as predicted with our classical Monte-Carlo simulations, based on the XCASCADE code. These simulations take into account the creation of laser-excited hot electrons and their elastic and inelastic collisions with ions. The model delivers the full temporal and spatial characteristics of the electron trajectories in various materials, including diamond and LiF. The comparison of the predicted electron range with the results of a recent XFEL experiment on LiF shows its reasonable agreement with the experimentally measured distribution of laser-generated color centers. In future, the code will be applied for simulations of hot carrier diffusion in X-ray-irradiated solids.

Primary authors:
Dr. LIPP, Vladimir (CFEL, DESY)

Co-authors :
Prof. ZIAJA-MOTYKA, Beata (CFEL, DESY)

Thermalization of hot XUV-generated electrons in diamond and LiF

Content:

We present the results of computer simulations

Primary authors:
Dr. LIPP, Vladimir (CFEL, DESY)

Co-authors :
Prof. ZIAJA-MOTYKA, Beata (CFEL, DESY)

Three-dimensional networks of interconnected ZnO and Cu2O nanowires fabricated by ion-track technology

Content:

Since a few decades, research on the synthesis and characterization of semiconductor nanowires has significantly increased, especially for sensor as well as energy applications such as solar cells and photoelectrochemical water splitting for hydrogen generation [1]. Combining ion-track technology and subsequent electrochemical deposition, we synthesize hierarchical ZnO [2] and p-Cu2O three-dimensional (3D) networks of highly interconnected nanowires. The fabrication of the etched ion-track membranes used as templates involves two separate processing steps: (i) Sequential irradiation of the template material from various directions with swift heavy ions and creation of latent tracks; (ii) selective ion-track dissolution and formation of interconnected channels by chemical etching. Control over the irradiation and etching conditions enables the production of various templates with channels of predefined geometries, sizes and aspect ratios.
Integration density and wire diameter are optimized in order to obtain mechanically stable and self-supporting 3D networks after dissolution of the polymer template [2, 3]. To increase their chemical stability the networks were subsequently coated with a thin amorphous TiO2 layer by atomic layer deposition (ALD). The optimal coating thickness was found to be between 10 and 20 nm. The homogeneity of the coated layer was confirmed by electron energy loss spectroscopy (EELS). The crystallinity of the TiO2 layer was investigated by high-resolution transmission electron microscopy (HRTEM) showing an anatase structure for deposition temperature as high as 250˚C, while the ALD at 110˚C resulted in an amorphous structure.
These nanowire networks were employed as model systems to study the photoelectrochemical performance of such hierarchical nanowire structures. The photoelectrochemical performance of these hierarchical 3D nanowire networks was compared to their film counterpart, showing a higher photocurrent for network-based photoelectrodes.
The reduced wire diameter, high surface-to-volume ratio, and the high degree of interconnectivity make these 3D systems very promising for photoelectrochemical cells due to the larger electrolyte-accessible surface area and the improved transport properties of the photogenerated charge carriers along highly crystalline wires of the networks.

[1] Hochbaum, A. I.; Yang, P. Chem. Rev. 110(1) (2010) 527.
[2] L. Movsesyan et al. Semicond. Sci. Technol. 31 (2016) 014006.
[3] M. Rauber, et. al., Nano Lett., 11 (2011) 2304-2310.

Primary authors:
MOVSESYAN, Liana (GSI Helmholtzzentrum für Schwerionenforschung)

Co-authors :
KUGELSTADT, Jan (GSI Helmholtzzentrum für Schwerionenforschung) Dr. YANG, Florent (GSI Helmholtzzentrum für Schwerionenforschung) Dr. MAIJENBURG, Wouter A. (GSI Helmholtzzentrum für Schwerionenforschung) Prof. TRAUTMANN, Christina (GSI Helmholtzzentrum für Schwerionenforschung) Dr. TOIMIL-MOLARES, Maria Eugenia (GSI Helmholtzzentrum für Schwerionenforschung)

Time resolved measurement of fluorescence kinetics from Adenine excited by soft X-rays

Content:

DNA shows a high stability against radiation damage. In order to prevent damaging chemical reactions there are pathways for a very fast decay of excited states created by radiation . By investigating the kinetics of UV-fluorescence excited by x-ray photons we want to contribute to the understanding of the molecular mechanisms behind the fast excitation decay.
For that purpose an experimental set-up to measure the fluorescence kinetics in the ps and sub-ps time range was developed using then up-conversion method. In first measurements of Adenine as an important constituent of DNA where X-ray absorption as well as ultra-fast relaxation processes take place a fast fluorescence decay in the ps time range was found.

Primary authors:
Dr. REDLIN, Harald (DESY / FS-LA)

Co-authors :
Dr. DZIARZHYTSKI, Siarhei (DESY / FS-FLASH-B) Dr. MALYI, Taras (University of Lviv, Ukraine) Dr. GERASIMOVA, Natalia (XFEL GmbH)

Time-resolved in-situ X-ray investigations during growth of InxGa1-xAs core-shell nanowire structures.

Content:

In the framework of a current BMBF funded project we are aiming to investigate the growth of semiconductor nanowires (NWs) by means of in-situ X-ray diffraction. We make use of a portable MBE chamber equipped with two Be-windows allowing for inspection of Bragg angles in a range between zero and 18 degree. Due to the compact design of the MBE chamber it can be mounted on common heavy load goniometers present at suitable synchrotron beamlines. Here we report on recent in-situ experiments performed at beamline P09 of PETRA III aiming at the nucleation, growth and elastic relaxation of an In0.25Ga0.75As shell growing on a Ga catalysed GaAs nanowire on Si(111) substrate. GaAs NWs were fabricated prior to the in-situ experiment and characterized by SEM to ascertain a known NW template suitable for growth of the shell. For GaAs growth a V/III ratio of FV/III=5 and a substrate temperature TS=590°C were used resulting in an axial growth rate of about 40 nm/min. At PETRA III the GaAs NW sample has been loaded into the pMBE again to study the InGaAs shell growth. In a first step the Ga droplet was consumed in As atmosphere to avoid continuation of axial growth. Subsequently, the shell was grown at TS=470°C and FV/III=4. The 2D layer growth rate was set to 45nm/h in order to be able to monitor the evolution of the shell by XRD.
The growth of the InGaAs shell was recorded by local reciprocal space maps around the symmetric (111) reflection and the asymmetric (311) and (220) zincblende and (10.3) wurtzite reflections. In all cases Si serves as a reference. The time resolution given by the duration of the scans is less than 3 min. High resolution maps of the whole reciprocal volume were done both at growth temperature and room temperature before and after finishing growth. The gradual appearance and evolution of InGaAs Bragg reflections has been successfully observed, detailed results will be shown during the presentation.

Primary authors:
Dr. FEIGL, Ludwig (Karlsruhe Institute of Technology (KIT), Institute for Photon Science and Synchrotron Radiation (IPS))

Topological quantum phase transition from weak to strong topological insulator

Content:

Time-reversal symmetry protects strong topological insulators of the Z2 class which possess an odd number of Dirac-cone surface states. Topological crystalline insulators are merely protected by individual crystal symmetries and are classified as weak topological insulators because of their even number of Dirac cones. Here we present measurements of the system Pb-Sn-Bi-Se which reveal a composition-dependent phase transition from topological crystalline insulator [1] to time-reversal-symmetry protected Z2 topological insulator and, therefore, from weak to strong. Moreover, a temperature-dependent phase transition from trivial to Z2 topological insulator is demonstrated.
For the class of topological crystalline insulators, it has early on been pointed out, that individual surface Dirac cones may be gapped at will by breaking of mirror symmetries [2]. By scanning-tunneling Landau-level spectroscopy [3,4] and ARPES [5] it has been seen that such an effect does occur at the (100) surface of Pb1-xSnxSe. It is important to note that in these cases, the topological phase remains unchanged by the symmetry-breaking distortion.
In principle, this does not need to be so: Distortions that lead to topological phase transitions have recently been predicted by density functional theory for two-dimensional TlSe [6] and three-dimensional SnTe [7]. In the present work, we investigate (111) epitaxial films of Pb-Sn-Bi-Se by angle-resolved photoemission and identify the Z2 topological insulator phase from a gapped Dirac cone at while the three cones at the M points remain intact. We interpret this as caused by a lattice distortion and suggest that the new Z2 phase is ferroelectric. This finding is highly interesting because it makes topological insulators in principle switchable electrically.
[1] P. Dziawa, B. J. Kowalski, K. Dybko, R. Buczko, A. Szczerbakow, M. Szot, E. Łusakowska, T. Balasubramanian, B. M. Wojek, M. H. Berntsen, O. Tjernberg, T. Story, Nat. Mater. 11, 1023 (2012).
[2] T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nat. Commun. 3, 982 (2012).
[3] Y. Okada, M. Serbyn, H. Lin, D. Walkup, W. Zhou, C. Dhital, M. Neupane, S. Xu, Y. J. Wang, R. Sankar, F. Chou, A. Bansil, M. Z. Hasan, S. D. Wilson, L. Fu, V. Madhavan, Science 341, 1496 (2013).
[4] I. Zeljkovic, Y. Okada, M. Serbyn, R. Sankar, D. Walkup, W. Zhou, J. Liu, G. Chang, Y. J. Wang, M. Z. Hasan, F. Chou, H. Lin, A. Bansil, L. Fu, V. Madhavan, Nat. Mater. 14, 318 (2015).
[5] B. M. Wojek, M. H. Berntsen, V. Jonsson, A. Szczerbakow, P. Dziawa, B. J. Kowalski, T. Story, O. Tjernberg, Nat. Commun. 6, 8463 (2015).
[6] C. Niu, P. M. Buhl, G. Bihlmayer, D. Wortmann, S. Blügel, Y. Mokrousov, Nano Lett. 15, 6071 (2015).
[7] E. Plekhanov, P. Barone, D. Di Sante, S. Picozzi, Phys. Rev. B 90, 161108(R) (2014).

Primary authors:
MANDAL, P.s. (Helmholtz-Zentrum Berlin, BESSY II, Albert Einstein Str. 15, 12489 Berlin, Germany)

Co-authors :
SPRINGHOLZ, G. (Institut for Semiconductor and Solid State Physics, JKU, Altenbergerstr. 69, 4040 Linz, Austria) BAUER, G. (Institut for Semiconductor and Solid State Physics, JKU, Altenbergerstr. 69, 4040 Linz, Austria) VOLOBUEV, V. V. (Institut for Semiconductor and Solid State Physics, JKU, Altenbergerstr. 69, 4040 Linz, Austria and National Technical University "KhPI", Frunze Str. 21, 61002 Kharkiv, Ukraine) CAHA, O. (Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic) VARYKHALOV, A. (Helmholtz-Zentrum Berlin, BESSY II, Albert Einstein Str. 15, 12489 Berlin, Germany) GOLIAS, E. (Helmholtz-Zentrum Berlin, BESSY II, Albert Einstein Str. 15, 12489 Berlin, Germany) RADER, O. (Helmholtz-Zentrum Berlin, BESSY II, Albert Einstein Str. 15, 12489 Berlin, Germany) SáNCHEZ-BARRIGA, J. (Helmholtz-Zentrum Berlin, BESSY II, Albert Einstein Str. 15, 12489 Berlin, Germany)

Tuning spin and charge order in geometrically frustrated rare earth ferrites

Content:

Rare earth ferrites RFe_2O_4 have attracted a lot of attention as prototypical examples of Multiferroics, which have a potential use in information technology in particular due to their proposed new mechanism of ferroelectricity arising from charge ordering (CO) of Fe^{2+} and Fe^{3+} in the Fe/O bilayers [1]. The $YbFe_2O_4$ exhibits a behavior very similar to $LuFe_2O_4$ [2], consistent with the primary importance of the rare earth ion size, which is comparable for both Yb^{3+} and Lu^{3+}. Alternatively, the Y^{3+} ionic radius is much larger, and a completely different charge order was found [3].

Given the completely different CO in $LuFe_2O_4$, and YFe_2O_4, it is of high interest to study "how charge and spin orders change while tuning the relevant interactions by gradually increasing the rare earth ion radius, made by substitution", i.e. the substitution $Lu_xY_{1-x}Fe_2O_4$. However, a critical aspect have to be considered in such a study is that, for each substitution level x, the oxygen-stoichiometry needs to be fine-tuned, as otherwise O-stoichiometry changes are impossible to cleanly disentangle from the rare earth substitution.

I will present results from substituting Y (larger ion size) by the smaller Lu i.e. $Lu_xY_{1-x}Fe_2O_4$, particularly for $X=0.5$. Polycrystalline $Lu_{0.5}Y_{0.5}Fe_2O_{4-\delta}$ quite close to the ideal stoichiometry was prepared for the first time and the magnetic behavior with only one main transition around 250 K contrasts with the behavior of YFe_2O_4 and is similar to that of $LuFe_2O_4$. Later on, the isothermal magnetization measurements show competing antiferromagnetic- ferrimagnetic phases, similar to $LuFe_2O_4$. Single crystals of $Lu_{0.5}Y_{0.5}Fe_2O_{4-\delta}$ grown under different CO_2/CO gas flows, were examined by single crystal x-ray diffraction showing 2D charge order with diffuse scattering along (1/3 1/3 l) even at low temperatures indicating that the crystals are not quite stoichiometric enough. Refinement of data from x-ray diffraction of powdered single crystals shows distinct changing in c-lattice parameter with gas ratio than YFe_2O_4 and $LuFe_2O_4$. As an outlook, further optimization is needed to verify that the charge and spin structures are indeed identical to $LuFe_2O_4$, indicated by the magnetic behavior of the polycrystalline sample.

[1] Ikeda et al., Nature 436, 1136 (2005).
[2] Williamson et al., unpublished.
[3] T. Mueller, J. de Groot, J. Strempfer, & M. Angst. Stoichiometric $YFe_2O_{4-\delta}$ single crystals, grown by the optical floating-zone method. J. Crystal Growth 428, 40 (2015).

Primary authors:
HAMMOUDA, Sabreen (Forschungszentrum juelich)

Ultra-doped Ge for optoelectronics: new perspectives of an old material

Content:

Independent of the type of doping, it is challenging to achieve in semiconductors an effective carrier concentration much above 1020 cm-3. On the other hand, the successful realization of defect free n-type and p-type ultra-doped Ge layers will enable a range of devices from sensors to quantum computers. In the case of conventional doping techniques (using equilibrium processing) the maximum carrier concentration is limited by the out-diffusion of dopants, a relatively low solid solubility limit, clustering and self-compensation processes. To overcome such limitations we have utilised strong nonequilibrium process consisting of an ion beam implantation to introduce dopants into Ge and rear-side millisecond range flash lamp annealing (FLA) for recrystallization of implanted layer and dopant activation. In contrast to conventional annealing procedures, rear-side FLA leads to full recrystallization of Ge and dopant activation independent of the pre-treatment. The maximum carrier concentration is well above 1020 cm-3 for n-type and above 1021 cm-3 for p-type dopants. The so-fabricated n-type Ge can be used in the field of mid-infrared plasmonics which has not been accessible by group-IV semiconductors. Single crystalline n-type Ge with carrier concentrations as high as 2.2×1020 cm-3 displays a room-temperature plasma frequency above 1850 cm-1 (λ=5.4 μm), which is the highest value ever reported for n-type Ge. In the case of Ga implanted Ge the maximum effective carrier concentration measured at 3K is 1.1×1021 cm-3 which is two times higher than the solid solubility limit of Ga in Ge. Our p-type Ge is defect and cluster free and shows the superconductivity at Tc = 0.95 K. These results base on the successful combination of ion beam implantation followed by the novel approach consisting of millisecond range rear-FLA.

Primary authors:
Dr. PRUCNAL, Slawomir (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Co-authors :
Dr. BERENCEN, Yonder (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany) Dr. ZHOU, Shengqiang (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany) Prof. HELM, Manfred (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany) Dr. SKORUPA, Wolfgang (Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany)

Ultra-fast solid-to-solid phase transition in diamond

Content:

Ultra-short FEL pulses at the FEL facilitiy FERMI were used to induce graphitization of diamond through a non-thermal solid-to-solid phase transition. This process was observed within poly-crystalline diamond in a time-resolved experiment and allowed the determination of this phase transition on a timescale of 150-200 fs. Excellent agreement between experiment and theoretical predictions were obtained using a dedicated code that follows non-equilibrium evolution of the irradiated diamond including all transient electronic and structural changes.

Primary authors:
Dr. TOLEIKIS, Sven (Deutsches Elektronen-Synchrotron DESY)

Co-authors :
Dr. TAVELLA, Franz (SLAC)

Ultrafast Water Heating at High XFEL Fluences

Content:

The bright ultrafast pulses of X-ray Free-Electron Lasers allow investigation into the structure of matter under extreme conditions. We have used these pulses to ionize and probe water as it undergoes a phase transition from liquid to plasma. We report changes in the structure of liquid water on a femtosecond timescale when irradiated by single 6.86 keV X-ray pulses of more than 106 J/cm2. These observations are supported by simulations based on molecular dynamics and plasma dynamics of a water system that is rapidly ionized and out of equilibrium. This unique ionically disordered state is suggested to be structurally different from a neutral thermally disordered state.

Primary authors:
Dr. BEYERLEIN, Kenneth (DESY CFEL)

Co-authors :
JOENSSON, Olof (Uppsala University) TIMNEANU, Nicusor (Uppsala University) CALEMAN, Carl (Uppsala University)

Ultrafast dynamics in transition metal dichalcogenides

Content:

Transition metal dichalcogenides have been widely studied since they exhibit a vast phase diagram including semi- and superconductivity, charge density waves as well as metal-to-insulator phase transitions. We present results of ultrafast dynamics in these systems investigated using a laser-pump x-ray probe setup as well as using the core-hole clock method. The former allows us to study dynamics from the femtosecond to the microsecond regime while using the latter we have access to the charge transfer times which happen on the sup-femtosecond regime.

Primary authors:
SORGENFREI, Florian (HZB)

Understanding the local structure of supercooled water via coherent x-ray scattering on liquid jets.

Content:

The anomalous physico-chemical properties of water, e.g. the density maximum at 4°C, are believed to arise from its strong hydrogen bonding network, which is much more pronounced in its supercooled state.[1] Thus, measuring the local arrangement of molecules in supercooled water and connecting it to its thermodynamic properties is one of the most fundamental questions in water research. Direct measurements of supercooled water in x-ray scattering and spectroscopy experiments can be quite challenging [2-5], and simulations have taken the lead in providing a link to water's microstructure-property relationship.[6] Using x-rays, one can readily calculate averaged pair correlation functions (or radial packing) of supercooled water [4], however, in these measurements, information relating to the instantaneous orientational order is smeared out due to the inherent temporal and spatial averaging process that takes place in conventional experiments in the lab or at storage rings.

Here, we will describe our efforts, where we (i) use a liquid jet system that breaks into micrometer sized droplets in vacuum, which then cool rapidly due to evaporation leading to water droplets in the supercooled regime, and
(ii) impinge these droplets with ultrashort (~ 100 fs at 120 Hz) coherent x-ray pulses at a Free-Electron Laser (FEL) source and thus, collect speckle patterns of these water droplets at different temperatures [7]. By using coherent x-rays, one can use angular cross-correlation methods [8] to estimate the mean orientation order. I will present our analysis efforts in this direction, and also provide parallels to the measurements with simulations of an ideal experiment with TIP4P/2005 water molecules.

[1] Lang, E. W. & Lüdemann, H. D. Angew. Chem. Int. Ed. 21 (1982);
[2] Bartell, L. & Huang, J. J. Phys. Chem. 98 (1994); Soper AK, Nat Mater. 13 (2014);
[3] T Head-Gordon & Hura G. Chem. Rev., 102 (2002); Sellberg JA et al., J. Chem. Phys.142 (2015);
[4] Sellberg JA et al. Nature 510, 381 (2014);
[5]. F. Lehmkühler, et al Phys. Chem. Chem. Phys. 18, 6925 (2016)
[6] Liu, Y., Palmer, J. C., Panagiotopoulos, A. Z. & Debenedetti, P. G. J. Chem. Phys. 137 (2012); Limmer, D. T. & Chandler, D. J. Chem. Phys. 135 (2011); Errington JR & Debenedetti PG. Nature 409 (2001);
[7] I. Steinke, et al. Rev. Sci. Instrum. 87, 6 (2016)
[8] Wochner P. et al. PNAS 106, 11511 (2009), F. Lehmkühler, et al. J. Appl. Crystallogr 47, 4 (2014); M. A. Schroer, et al. Soft Matter 11, 27 (2015)

Primary authors:
Dr. JAIN, Avni (DESY, Hamburg)

Co-authors :
Dr. GRUEBEL, Gerhard (DESY, Hamburg)

Unravelling the mechanism of the magnetocaloric effect in Mn5Si3

Content:

The search for more efficient use of energy has been leading to a growing interest for the research field of magnetocaloric materials. The magnetocaloric effect (MCE) refers to a change of temperature or entropy of a magnetic material exposed to a change of magnetic field.
The MCE requires the exchange of magnetic entropy, lattice entropy and/or electronic entropy during the adiabatic (de-)magnetization process.

A large MCE and low magnetic field for a material with abundant and environmentally friendly elements opens the way for magnetic cooling devices.
The system Mn5-xFexSi3 shows a modestly large MCE close to room temperature at low magnetic fields, which is promising for magnetic refrigeration applications.
In order to investigate the underlying mechanisms of magnetocaloric materials (MCM), we need to understand the nature of magnetism (itinerant or localized) and the coupling between the spin and lattice degrees of freedom.

The parent compound Mn5Si3 has been extensively characterized by magnetometry, X-ray and neutron diffraction.
It exhibits the inverse-MCE (the sample cools down when the external magnetic field is applied adiabatically) and evidence of the direct-MCE (the sample heats up when the external magnetic field is applied adiabatically) in relation with two distinct magnetic phase transitions at TN1=66 K (non-collinear antiferromagnetic AF1 phase) and TN2=99 K (collinear antiferromagnetic AF2 phase), respectively.
In the collinear phase moments order on only one Mn site out of the three distinct crystallographic Mn sites.
In the non-collinear phase Mn atoms order for 2 of the 3 crystallographic sites in a non-collinear and non-coplanar structure.

Inelastic neutron scattering experiments were performed in the paramagnetic and the different magnetically ordered phases where a markedly different spin excitation spectrum is found.
At lower temperatures within the AF1 phase strong spin waves are characteristic where at higher temperatures within the AF2 phase an evidence of strong magnetic fluctuations are found in coexistence with well-defined spin waves.
These fluctuations could play an essential role in the MCE.
Further studies on spin and lattice dynamics also in magnetic field might help to unravel the microscopic mechanism of the MCE.

Primary authors:
Dr. SCHMALZL, Karin (JCNS, Forschungszentrum Juelich GmbH, Outstation at ILL, Grenoble, France) Mr. BINISKOS, Nikolaos (JCNS, Forschungszentrum Juelich GmbH, Outstation at ILL, and CEA Grenoble, INAC MEM, 38054 Grenoble, France)

Co-authors :
Dr. RAYMOND, Stephane (Université Grenoble Alpes and CEA Grenoble, INAC MEM, 38054 Grenoble, France) Dr. PETIT, Sylvain (Laboratoire Léon Brillouin, CEA-CNRS, CEA-Saclay, F-91191 Gif-sur-Yvette, France) PERSSON, Joerg (Juelich Centre for Neutron Science and Peter Gruenberg Institut PGI, JARA-FIT, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany) Prof. BRUECKEL, Thomas (Juelich Centre for Neutron Science and Peter Gruenberg Institut PGI, JARA-FIT, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany)

Unusual Coulomb scattering processes in graphene

Content:

Graphene, the two-dimensional allotrope of carbon, is characterized by a gapless linear band structure. This unique band structure is directly related to some unusual phenomena regarding the ultrafast Coulomb dynamics in the material. The understanding of this dynamics is of vital interest, both from a fundamental as well as from an application oriented point of view. The elastic Coulomb scattering is the main mechanism for thermalization of a non-equilibrium carrier distribution.
We investigate the carrier dynamics in a regime, where scattering via optical phonons is strongly suppressed. To this end, time resolved spectroscopy was performed with radiation of photon energies around 75 meV, which is smaller than the optical phonon energy (~200 meV). In polarization resolved experiments using co- and cross-polarized linearly polarized pump and probe beams, respectively, the Coulomb scattering dynamics is investigated. We find a two-fold nature of this process, namely very fast (fs timescale) collinear Coulomb scattering but surprisingly slow (ps-timescale) non-collinear scattering [1].
In the presence of a magnetic field, the linear band structure of graphene splits up into a series of non-equidistant Landau levels. Studying the transitions between the lowest Landau levels in pump-probe and four-wave mixing experiments, we find evidence for strong Auger scattering [2, 3].

[1] J. C. König-Otto, M. Mittendorff, T. Winzer, F. Kadi, E. Malic, A. Knorr, C. Berger, W. A. de Heer, A. Pashkin, H. Schneider, M. Helm, and S. Winnerl, Phys. Rev. Lett. 117, 087401 (2016).

[2] M. Mittendorff, F. Wendler, E. Malic, A. Knorr, M. Orlita, M. Potemski, C. Berger, W. A. de Heer, H. Schneider, M. Helm, and S. Winnerl, Nature Phys. 11, 75 (2015).

[3] J. C. König-Otto, Y. Wang, A. Belyanin, C. Berger, W. A. de Heer, M. Orlita, A. Pashkin, H. Schneider, M. Helm, and S. Winnerl (submitted).

Primary authors:
Dr. WINNERL, Stephan (Helmholtz-Zentrum Dresden-Rossendorf)

Co-authors :
Mr. KöNIG-OTTO, Jacob (HZDR) Dr. PASHKIN, Alexej (HZDR) Dr. SCHNEIDER, Harald (HZDR) Prof. HELM, Manfred (HZDR)

VEKMAG - a vector magnet for BESSY II

Content:

We present the VEKMAG end station which includes a vector superconducting magnet a deposition chamber and an advanced detector system, which has been jointly developed by Universität Regensburg, Freie Universität Berlin, Ruhr-Universität Bochum, and Helmholtz-Zentrum Berlin. The instrument is since recently in user operation at the PM2 dipole beamline of the synchrotron facility BESSY II in Berlin, offering circularly polarized soft x-rays between 20 eV and 1600 eV with a variable focus size. The instrument is designed for research of future spintronic materials for information technology, such as multi and single-layer magnetic thin films, nanostructures, molecules as well as some complex single crystals materials. Experimental probes include XAS, XMCD/XMLD measurements, resonant soft X-ray scattering methods, as well as time-resolved ferromagnetic resonance (FMR) and electron paramagnetic resonance (EPR) using XMCD. The available temperature range extends from 2. K up to 500 K. It provides a 9 T field in the beam direction, a 2 T field in the horizontal plane, and a 1 T field perpendicular direction. These fields can be operated on single axis but also in a vectorial manner. Some selected results are presented to show the capabilities of the instrumentation.

Primary authors:
Dr. RADU, Florin (Helmholtz-Zentrum Berlin)

Co-authors :
RYLL, H. () LUO, C. () ABRUDAN, R. () RUDORFF, S. () RADER, O. () NOLL, T. () KUCH, W. () BRITTON, A.j. () MACHADO-ARRUGA, L. () ZABEL, H. () WOLTERSDORF, G. () BACK, C. ()

Vicinal ZnO(10-14): surface structure and stability

Content:

Zinc oxide (ZnO) based catalysts are commonly used in important chemical reactions as methanol synthesis (CO + 2H2 ⇆ CH3OH), low temperature water-gas shift (CO + H2O ⇆ CO2 +H2), and methanol steam reforming (CH3OH + H2O ⇆ CO2 + 3H2O) [1]. Determination of the stable ZnO surface structure and studies of how it interacts with the gases is essential for understanding catalytic processes.
The commonly studied (0001) and (000-1) orientations of ZnO are both polar, resulting in instability of these surfaces. Stabilization of the ZnO(0001) surface has recently been suggested to occur through faceting into large areas of the charge neutral, high step-density, vicinal (10-14) surface [2]. The interaction between steps on vicinal surfaces plays a crucial role for the equilibrium structure, and very little is still known about the equilibrium structure of vicinal oxide surfaces. Here we will present studies of the clean ZnO(10-14) surface using techniques such as low-energy electron diffraction, x-ray photoelectron spectroscopy, and scanning probe microscopy.
Further, the interaction of such a vicinal surface with the gases involved in the catalytic reactions is of uttermost importance. In a first step towards understanding the catalytic role of vicinal ZnO we have studied H2O exposure of the ZnO(10-14) surface. Here we will show some initial results from these studies.

[1] C. Wöll, Progress in Surface Science 82, 55-120 (2007)
[2] H. Zheng, et al., Phys. Rev. Lett. 111, 086101 (2013)

Primary authors:
Dr. GRåNäS, Elin (DESY NanoLab, Hamburg, Germany)

Co-authors :
Mr. ARNDT, Björn (DESY NanoLab and Hamburg University, Hamburg, Germany) Mr. CREUTZBURG, Marcus (DESY NanoLab and Hamburg University, Hamburg, Germany) Mr. DALLA LANA SEMIONE, Guilherme (DESY NanoLab and Hamburg University, Hamburg, Germany) Dr. NOEI, Heshmat (DESY NanoLab, Hamburg, Germany) Dr. SCHAEFER, Andreas (Synchrotron Radiation Research, Department of Physics, Lund University, Lund, Sweden) Dr. GUSTAFSON, Johan (Synchrotron Radiation Research, Department of Physics, Lund University, Lund, Sweden) Dr. VONK, Vedran (DESY NanoLab, Hamburg, Germany) Prof. STIERLE, Andreas (DESY NanoLab and Hamburg University, Hamburg, Germany)

Water Window Ptychographic Imaging of Biological Samples

Content:

X-ray ptychography is a diffractive imaging technique to obtain large field of view reconstructions of objects on a high resolution level. Although hard X-rays (between 7 keV and 13 keV) provide less complicated experimental access to micro-structure determination, the soft X-ray range of the water window (284 eV to 532 eV) offers unique imaging opportunities. Here a maximum of contrast between biological and its aqueous components can be obtained without any additional contrast enhancing sample preparation. Thus a cell stays in its most natural state promising insight into its undisturbed nano-structure. We have collected a high resolution soft X-ray ptychographic diffraction data set of a dried and unstained fibroblast cell. By using a beam stop and two exposures we have effectively extended the dynamical range of the collected diffraction data which gives access to water window imaging of biological objects. Here we present new results on a high resolution X-ray imaging experiment of a biological fibroblast cell and our strategy for radiation damage limited resolution water window ptychography.

Primary authors:
Mr. ROSE, Max (PIER Fellow)

X-ray imaging application at the multi-contrast laboratory setup at IPS

Content:

This poster deals with our three possible setups for life science research at the multi-contrast laboratory of the Institute for Photon Science and Synchrotron Radiation. In particular we present a method called augmented laminography and show an application for flat extended fossils. Furthermore we demonstrate our ability to exam biological samples with micro-CT and grating interferometry.

Primary authors:
Mr. ZUBER, Marcus (Karlsruhe Institute of Technology)

Co-authors :
Ms. ENGELHARDT, Sabine (Karlsruhe Institute of Technology) Dr. HAMANN, Elias (Karlsruhe Institute of Technology) Dr. VAN DE KAMP, Thomas (Karlsruhe Institute of Technology) Prof. TILO, Baumbach (Karlsruhe Institute of Technology)

X-ray imaging for developmental biology

Content:

The development of sophisticated imaging techniques was a major driving force for the tremendous progress in life science, especially in developmental biology, over the past years. In the last two decades, there has been great progress in the development of new imaging techniques as well as great advance in already existing techniques. A common downside of established imaging techniques like light sheet microscopy, multi photon microscopy or electron microscopy is that specimens have to be transparent and of relatively small dimensions. Due to these limitations, mechanical sectioning of organs or tissues is required for imaging. Recent developments in X-ray imaging techniques together with our expertise on X-ray imaging techniques in life science grant us a new way of looking at model organisms. X-rays are known for their capability to penetrate thick and opaque tissues, providing a complete tomographic view of electron dense materials even within large specimen. The protocols, established within recent projects in the host laboratories, provide high resolution tomographic data of entire animals by imparting X-ray contrast to soft tissue, otherwise transparent to X-rays, making possible in vivo 4-D imaging.

Primary authors:
Dr. WEINHARDT, Venera (Institute for Photon Science and Synchrotron Radiation)

Co-authors :
Dr. HOFMANN, Talf (Institute for Photon Science and Synchrotron Radiation) Dr. BAUMBACH, Tilo (Institute for Photon Science and Synchrotron Radiation) Dr. WITTBRODT, Jochen (Centre for Organismal Studies, Heidelberg University) Dr. LOOSLI, Felix (Institute of Texicology and Genetics, KIT)

X-ray induced dynamics in matter: from finite towards macroscopic systems

Content:

High intensity X-ray Free Electron Lasers (XFEL) revolutionize the experimental capabilities in the field of exploring molecular and atomic matter. The extreme properties of the XFEL pulses allow one to look into dynamics happening on femtosecond timescales and at atomic length scales even in systems of size down to a singe atom. During a high intensity measurement the x-rays alter the target. Theoretical understanding of such induced dynamics is crucial for both planning experiments and interpreting measured data.

We present recent results based on Molecular Dynamics simulations. Rich spectroscopic data on finite systems, e.g. on clusters can be experimentally collected. However, more insight into the time evolution could be gained through modeling only, revealing the role of the microscopic driving processes. Further, due to an extension of our code it is possible to simulate extended bulk matter. We use this latter capability in the theoretical investigations of nanocrystal imaging and of the dynamics of warm dense matter.

Primary authors:
Dr. JUREK, Zoltan (CFEL, DESY) Mr. ABDULLAH, Malik Muhammad (CFEL, DESY) Dr. TOYOTA, Koudai (CFEL, DESY) Dr. SON, Sang-kil (CFEL, DESY) Prof. ZIAJA, Beata (CFEL, DESY) Prof. SANTRA, Robin (CFEL, DESY)

X-ray quantum optics in thin-film nanostructures

Content:

Quantum optics is one of the most active and important fields of modern physics, encompassing all experiments where the interaction of light and matter is manipulated. Although the majority of experiments have been performed with visible light and microwaves, recent years have seen an extension to the spectral range of hard x-rays. This has mostly been achieved through the use of thin films with nuclear and electronic resonances. We give a brief overview over this rapidly developing field, sketching some of the more recent successes, including the observation of strong coupling, Rabi oscillations and collective Lamb shifts. We also discuss likely future developments.

Primary authors:
HABER, Johann (DESY) RöHLSBERGER, Ralf (DESY)

Co-authors :
GOLLWITZER, Jakob (DESY) WILLING, Svenja (DESY) BOCKLAGE, Lars (DESY) SCHLAGE, Kai (DESY) SCHULZE, Kai-sven (Helmholtz-Institut Jena) GERNHARDT, Robert (Helmholtz-Institut Jena) PAULUS, Gerhard G. (Universität Jena) BERNHARDT, Hendrik (Universität Jena)

^[77]Se NMR on single crystalline FeSe

Content:

FeSe is currently discussed as a superconductor in the crossover regime between the weakly coupled Bardeen-Cooper-Schrieffer (BCS) and the strongly coupled Bose-Einstein-condensate (BEC) limit. In particular, at elevated magnetic fields, the energies of the Zeeman interaction, superconducting gap, and the Fermi temperature are comparable in this material. We report recent results of the spin susceptibility and low-energy quasiparticle excitations probed by means of nuclear magnetic resonance (NMR) spectroscopy in the highly spin-polarized state close to the upper critical field of superconductivity.

Primary authors:
Mr. MOLATTA, Sebastian (Hochfeld-Magnetlabor Dresden (HLD-EMFL))

Co-authors :
Dr. ZHANG, Z. T. (Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany) Dr. SARKA, R. (Dresden University of Technology, Department of Physics, 01062 Dresden, Germany) Dr. BISWAS, P. (Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institut, 5232 Villigen, Switzerland) Dr. WOLF, T. (Karlsruhe Institute of Technologie, Department of Physics, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany) Prof. LöHNEYSEN, H. V. (Karlsruhe Institute of Technologie, Department of Physics, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany) Prof. WOSNITZA, J. (Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany 2) Dresden University of Technology, Department of Physics, 01062 Dresden, Germany) Dr. KüHNE, H. (Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany 2) Dresden University of Technology, Department of Physics, 01062 Dresden, Germany)