On the interpretation of Mössbauer spectra of magnetic nanoparticles

Mössbauer spectra of magnetic nanoparticles are usually influenced by fluctuations of the direction of the magnetic hyperfine field. In samples of non-interacting particles, the superparamagnetic relaxation usually results in spectra consisting of a sum of a sextet and a doublet with a temperature dependent area ratio. This is in accordance with the exponential dependence of the superparamagnetic relaxation time on particle size and temperature in combination with the particle size distribution. An alternative interpretation of these features is a first order magnetic transition from a magnetically ordered state to a paramagnetic state. We point out that this interpretation seems not to be correct, because the doublet component has been found to transform to a magnetically split component when relatively small magnetic fields are applied, and therefore it cannot be due to a paramagnetic state. In other cases, spectra of magnetic nanoparticles consist of sextets with asymmetrically broadened lines without the presence of doublets. It has been suggested that such spectra can be explained by a multilevel model, according to which relaxation takes place between a large number of states. We point out that spectra with asymmetrically broadened lines at least in some cases rather should be explained by the influence of magnetic inter-particle interactions on the magnetic fluctuations.
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.71 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.756 SNIP 1.391 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.821 SNIP 1.435 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.807 SNIP 1.4 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.929 SNIP 1.302 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.068 SNIP 1.285 CiteScore 1.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.916 SNIP 0.973
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.846 SNIP 0.916
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.861 SNIP 0.897
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.708 SNIP 0.848
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.832 SNIP 0.877
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.683 SNIP 0.693
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.792 SNIP 1.037
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.975 SNIP 0.897
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.188 SNIP 1.079
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.139 SNIP 0.952
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.19 SNIP 0.935
Web of Science (2000): Indexed yes
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57Fe-Mössbauer spectroscopy and electrochemical activities of graphitic layer encapsulated iron electrocatalysts for the oxygen reduction reaction

Graphitic layer encapsulated iron based nanoparticles (G@FeNPs) have recently been disclosed as an interesting type of highly active electrocatalysts for the oxygen reduction reaction (ORR). However, the complex composition of the metal-containing components and their contributions in catalysis remain unclear. As a representative catalyst of the unique encapsulated structure, a series of G@FeNPs catalysts were prepared by a high-pressure pyrolytic process with uniform and essentially identical morphologies but varied compositions. The catalysts exhibited a high onset potential of 0.85 V at 0.1 mA cm⁻² in acidic media. By 57Fe-Mössbauer spectroscopy the iron containing components were identified including α-Fe, γ-Fe, γ-Fe₂O₃, and Fe₃C as well as a minor doublet component due to Fe³⁺ in high spin and/or Fe²⁺ in low spin state. The ORR activities are evaluated in terms of the mass specific kinetic current density found to be positively correlated with the Fe₃C content in the range of study, indicating involvement of the encapsulated nanoparticles in the ORR catalysis. The recognition of the Fe compositions and active sites provides new insights to the confined Fe-based ORR electrocatalysts and therefore options for further development of non-precious metal materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Neutrons and X-rays for Materials Physics, Proton conductors
Authors: Zhong, L. (Intern), Frandsen, C. (Intern), Mørup, S. (Intern), Hu, Y. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.583 SNIP 2.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.26 SNIP 2.081 CiteScore 7.72
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.232 SNIP 2.164 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.345 SNIP 2.134 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.629 SNIP 2.236 CiteScore 6.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.585 SNIP 2.345 CiteScore 6.14
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.461 SNIP 1.895
Web of Science (2010): Indexed yes
HIGH PRECISION COMPUTED TOMOGRAPHY FOR METROLOGY

Disclosed is a CT system for performing measurements on an object. The CT system comprises a support element for supporting the object; a radiation source for radiating the object at a plurality of different angles; a radiation detector assembly for detecting radiation passed through the object and in response thereto generate radiation data; and a processing unit operatively connected to the radiation detector assembly. The radiation detector assembly comprises a support, a first detector array, and a second detector array, the first detector array and the second detector array being attached to the support. The processing is configured to generate tomographic images of the object by processing radiation data received from the radiation detector assembly together with first calibration data describing properties of the first detector array and second calibration data describing properties of the second detector array.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Gundlach, C. (Intern), Poulsen, H. F. (Intern)
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Electronic versions:
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Main Research Area: Technical/natural sciences
Source: espacenet
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A METHOD OF SECURITY SCANNING OF CARRY-ON ITEMS, AND A CARRY-ON ITEMS SECURITY SCANNING SYSTEM

A security scanning system (1) comprises a first stage module (3) having at least one X-ray source (6) and at least three first detectors (7) that are line-shaped and arranged in mutually different orientations and have at least dual energy resolution. A group of carry-on items (4) on a carrier are scanned simultaneously in the first stage module solely by transmission contrast radiography generating projections of two-dimensional image data. A processing device (9) reconstructs a 3D representation of the carry-on items and analyzes the 3D representation to determine whether further scanning is required.

Alloy design as an inverse problem of cluster expansion models

Central to a lattice model of an alloy system is the description of the energy of a given atomic configuration, which can be conveniently developed through a cluster expansion. Given a specific cluster expansion, the ground state of the lattice model at 0 K can be solved by finding the configuration of solutes that minimizes the energy of the system. In this paper, we develop a method for solving the inverse lattice problem, where, given a broad class of potential, we find the ground states for all possible values of the effective cluster interaction energies. To do so, we formulate the inverse problem in terms of energetically distinct configurations, using a constraint satisfaction model to identify constructible configurations, and show that a convex hull can be used to identify ground states. To demonstrate the approach, we solve for all ground states for a binary alloy in a 2D hexagonal lattice both with and without an interface, based on pairwise interactions.
A low-spin Fe(III) complex with 100-ps ligand-to-metal charge transfer photoluminescence

Transition-metal complexes are used as photosensitizers(1), in light-emitting diodes, for biosensing and in photocatalysis(2). A key feature in these applications is excitation from the ground state to a charge-transfer state(3,4); the long charge-transfer-state lifetimes typical for complexes of ruthenium(5) and other precious metals are often essential to ensure high performance. There is much interest in replacing these scarce elements with Earth-abundant metals, with iron(6) and copper(7) being particularly attractive owing to their low cost and non-toxicity. But despite the exploration of innovative molecular designs(6,8-10), it remains a formidable scientific challenge(11) to access Earth-abundant transition-
metal complexes with long-lived charge-transfer excited states. No known iron complexes are considered(12) photoluminescent at room temperature, and their rapid excited-state deactivation precludes their use as photosensitizers(13-15). Here we present the iron complex [Fe(btz)(3)](3+) (where btz is 3,3'-dimethyl-1,1'-bis(p-tolyl)-4,4'-bis(1,2,3-triazol-5-yldiene)), and show that the superior sigma-donor and pi-acceptor electron properties of the ligand stabilize the excited state sufficiently to realize a long charge-transfer lifetime of 100 picoseconds (ps) and room-temperature photoluminescence. This species is a low-spin Fe(III) d(5) complex, and emission occurs from a long-lived doublet ligand-to-metal charge-transfer ((LMCT)-L-2) state that is rarely seen for transition-metal complexes(4,16,17). The absence of intersystem crossing, which often gives rise to large excited-state energy losses in transition-metal complexes, enables the observation of spin-allowed emission directly to the ground state and could be exploited as an increased driving force in photochemical reactions on surfaces. These findings suggest that appropriate design strategies can deliver new iron-based materials for use as light emitters and photosensitizers.

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Scopus rating (2016): CiteScore 13.33
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.22
Web of Science (2014): Indexed yes
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Scopus rating (2013): CiteScore 14.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 14.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
A Monte Carlo simulation of scattering reduction in spectral X-ray computed tomography

In X-ray computed tomography (CT), scattered radiation plays an important role in the accurate reconstruction of the inspected object, leading to a loss of contrast between the different materials in the reconstruction volume and cupping artifacts in the images. We present a Monte Carlo simulation tool for spectral X-ray CT to predict the scattered radiation generated by complex samples. An experimental setup is presented to isolate the energy distribution of scattered radiation. Spectral CT is a novel technique implementing photon-counting detectors able to discriminate the energy of incoming photons, enabling spectral analysis of X-ray images. This technique is useful to extract efficiently more information on energy dependent quantities (e.g. mass attenuations coefficients) and study matter interactions (e.g. X-ray scattering, photoelectric absorption, etc...). Having a good knowledge of the spectral distribution of the scattered X-rays is fundamental to establish methods attempting to correct for it. The simulations are validated by real measurements using a CdTe spectral resolving detector (Multix ME-100). We observed the effect of the scattered radiation on the image reconstruction, becoming relevant in the energy range where the Compton events are dominant (i.e. above 50keV).

Coherent structural trapping through wave packet dispersion during photoinduced spin state switching

The description of ultrafast nonadiabatic chemical dynamics during molecular photo-transformations remains challenging because electronic and nuclear configurations impact each other and cannot be treated independently. Here we gain experimental insights, beyond the Born-Oppenheimer approximation, into the light-induced spin-state trapping dynamics of the prototypical [Fe(bpy)]_3^{2+} compound by time-resolved X-ray absorption spectroscopy at sub-30-femtosecond
resolution and high signal-to-noise ratio. The electronic decay from the initial optically excited electronic state towards the high spin state is distinguished from the structural trapping dynamics, which launches a coherent oscillating wave packet (265 fs period), clearly identified as molecular breathing. Throughout the structural trapping, the dispersion of the wave packet along the reaction coordinate reveals details of intramolecular vibronic coupling before a slower vibrational energy dissipation to the solution environment. These findings illustrate how modern time-resolved X-ray absorption spectroscopy can provide key information to unravel dynamic details of photo-functional molecules.
Colloidal Flower-Shaped Iron Oxide Nanoparticles: Synthesis Strategies and Coatings

The assembly of magnetic cores into regular structures may notably influence the properties displayed by a magnetic colloid. In this work, key synthesis parameters driving the self-assembly process capable of organizing colloidal magnetic cores into highly regular and reproducible multi-core nanoparticles are determined. In addition, a self-consistent picture that explains the collective magnetic properties exhibited by these complex assemblies is achieved through structural, colloidal, and magnetic means. For this purpose, different strategies to obtain flower-shaped iron oxide assemblies in the size range 25–100 nm are examined. The routes are based on the partial oxidation of Fe(OH)$_2$, polyol-mediated synthesis or the reduction of iron acetylacetonate. The nanoparticles are functionalized either with dextran, citric acid, or alternatively embedded in polystyrene and their long-term stability is assessed. The core size is measured, calculated, and modeled using both structural and magnetic means while the Debye model and multi-core extended model are used to study interparticle interactions. This is the first step toward standardized protocols of synthesis and characterization of flower-shaped nanoparticles.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Micro- and Nanotechnology, Magnetic Systems, Instituto de Ciencia de Materiales de Madrid, Micromod Partikeltechnologie GmbH, nanoPET Pharma GmbH, SP Technical Research Institute of Sweden, UCL Healthcare Biomagnetics Laboratory, Physikalisch-Technische Bundesanstalt, Chalmers University of Technology, University of Cantabria, Technische Universität Braunschweig, Uppsala University
Number of pages: 12
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Main Research Area: Technical/natural sciences
Damped spin excitations in a doped cuprate superconductor with orbital hybridization

A resonant inelastic x-ray scattering study of overdamped spin excitations in slightly underdoped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) with $x = 0.12$ and $0.145$ is presented. Three high-symmetry directions have been investigated: (1) the antinodal (0,0) -> (½,0), (2) the nodal (0,0) -> (¼, ¼), and (3) the zone-boundary direction (½,0) -> (¼, ¼) connecting these two. The overdamped excitations exhibit strong dispersions along (1) and (3), whereas a much more modest dispersion is found along (2). This is in strong contrast to the undoped compound La$_2$CuO$_4$ (LCO) for which the strongest dispersions are found along (1) and (2). The $t$ - $t'$ - $t''$ - $U$ Hubbard model used to explain the excitation spectrum of LCO predicts for constant $U/t$ that the dispersion along (3) scales with $(t'/t)^2$. However, the diagonal hopping $t'$ extracted on LSCO using single-band models is low ($t'/t \sim -0.16$) and decreasing with doping. We therefore invoked a two-orbital ($d_{x^2-y^2}$ and $d_{z^2}$) model which implies that $t'$ is enhanced. This effect acts to enhance the zone-boundary dispersion within the Hubbard model. We thus conclude that hybridization of $d_{x^2-y^2}$ and $d_{z^2}$ states has a significant impact on the zone-boundary dispersion in LSCO.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Universität Zürich, Ecole Polytechnique Federale de Lausanne (EPFL), Paul Scherrer Institut, University of Central Lancashire, Hokkaido University
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Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
Determination of low-strain interfaces via geometric matching

We present a general method for combining two crystals into an interface. The method finds all possible interfaces between the crystals with small coincidence cells and identifies the strain and area of the corresponding two-dimensional cells of the two crystal surfaces. We apply the method to the two semiconductor alloys In$_{1-x}$Sb$_x$ and Ga$_{1-x}$In$_x$As combined with a selection of pure metals or with NbTiN to create semiconductor/superconductor interfaces. The lattice constant of the alloy can be tuned by composition and we can extract the alloy lattice parameters corresponding to zero strain in both the metal and the alloy. The results can be used to suggest new epitaxially matched interfaces between two materials.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Neutrons and X-rays for Materials Physics, QuantumWise A/S
Authors: Jelver, L. (Intern), Larsen, P. M. (Intern), Stradi, D. (Ekstern), Stokbro, K. (Ekstern), Jacobsen, K. W. (Intern)
Number of pages: 7
Publication date: 2017
Determining material parameters using phase-field simulations and experiments

A method to determine material parameters by comparing the evolution of experimentally determined 3D microstructures to simulated 3D microstructures is proposed. The temporal evolution of a dendritic solid-liquid mixture is acquired in situ using x-ray tomography. Using a time step from these data as an initial condition in a phase-field simulation, the computed structure is compared to that measured experimentally at a later time. An optimization technique is used to find the material parameters that yield the best match of the simulated microstructure to the measured microstructure in a global manner. The proposed method is used to determine the liquid diffusion coefficient in an isothermal Al-Cu alloy. However, the method developed is broadly applicable to other experiments in which the evolution of the three-dimensional microstructure is determined in situ. We also discuss methods to describe the local variation of the best-fit parameters and the fidelity of the fitting. We find a liquid diffusion coefficient that is different from that measured using directional solidification.
Effect of carbon on interstitial ordering and magnetic properties of $\varepsilon$-Fe$_2$(N,C)$_{1-z}$

Hexagonal $\varepsilon$-iron nitride and $\varepsilon$-iron carbonitride phases are formed on nitriding and nitrocarburizing of iron and steel surfaces and can exist in broad compositional ranges. Long-range nitrogen ordering and magnetic properties for $\varepsilon$-iron nitrides and their dependence on composition have been the focus of several studies. So far, limited attention has been paid to the carbonitrides. In the current work, the effects of substitution of nitrogen by carbon on the interstitial ordering and magnetic properties in Fe$_2$(C,N)$_{1-z}$ are explored using neutron diffraction, Mössbauer spectroscopy and vibrating sample magnetometry. Neutron diffraction patterns showed 001 and 301 superstructure reflections, confirming a previously proposed structural model in space group P31m (compared to P6$_3$22 for the pure nitrides). On partial substitution of nitrogen by carbon in $\varepsilon$-iron nitride the Curie temperature, the saturation magnetization and the hyperfine fields of the iron atoms are increased, while isomer shifts are decreased. The effects on the a and c lattice parameters indicate a change in interstitial ordering, which is related to more favorable interactions between a nitrogen and carbon atom than among nitrogen atoms. This interaction leads to additional interstitial (short-range) ordering and a decrease in the c lattice parameter, while the a lattice parameter is largely unaffected.
Electromechanical Response of Polycrystalline Barium Titanate Resolved at the Grain Scale

Ferroic materials are critical components in many modern devices. Polycrystalline states of these materials dominate the market due to their cost effectiveness and ease of production. Studying the coupling of ferroic properties across grain boundaries and within clusters of grains is therefore critical for understanding bulk polycrystalline ferroic behavior. Here, three-dimensional X-ray diffraction is used to reconstruct a 3D grain map (grain orientations and neighborhoods) of a polycrystalline barium titanate sample and track the grain-scale non-180° ferroelectric domain switching strains of 139 individual grains in situ under an applied electric field. The map shows that each grain is located in a very unique local environment in terms of intergranular misorientations, leading to local strain heterogeneity in the as-processed state of the sample. While primarily dependent on the crystallographic orientation relative to the field directions, the response of individual grains is also heterogeneous. These unique experimental results are of critical importance both when building the starting conditions and considering the validity of grain-scale modeling efforts, and provide additional considerations in the design of novel ferroic materials.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility
Authors: Majkut, M. (Intern), Daniels, J. E. (Ekstern), Wright, J. P. (Ekstern), Schmidt, S. (Intern), Oddershede, J. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1 SNIP 1.369
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.017 SNIP 1.42 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.192 SNIP 1.628 CiteScore 2.78
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.168 SNIP 1.481 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
FELIX: an algorithm for indexing multiple crystallites in X-ray free-electron laser snapshot diffraction images

A novel algorithm for indexing multiple crystals in snapshot X-ray diffraction images, especially suited for serial crystallography data, is presented. The algorithm, FELIX, utilizes a generalized parametrization of the Rodrigues-Frank space, in which all crystal systems can be represented without singularities. The new algorithm is shown to be capable of indexing more than ten crystals per image in simulations of cubic, tetragonal and monoclinic crystal diffraction patterns. It is also used to index an experimental serial crystallography dataset from lysozyme microcrystals. The increased number of indexed crystals is shown to result in a better signal-to-noise ratio, and fewer images are needed to achieve the same data quality as when indexing one crystal per image. The relative orientations between the multiple crystals indexed in an image show a slight tendency of the lysozme microcrystals to adhere on (110) facets.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Neutrons and X-rays for Materials Physics, Theoretical Atomic-scale Physics, Deutsches Elektronensynchrotron DESY
Authors: Beyerlein, K. R. (Ekstern), White, T. A. (Ekstern), Yefanov, O. (Ekstern), Gati, C. (Ekstern), Kazantsev, I. G. (Intern), Gade-Nielsen, N. F. (Intern), Larsen, P. M. (Intern), Chapman, H. N. (Ekstern), Schmidt, S. (Intern)
Field-induced reentrant magnetoelectric phase in LiNiPO₄

Using pulsed magnetic fields up to 30 T we have measured the bulk magnetization and electrical polarization of LiNiPO₄ and have studied its magnetic structure by time-of-flight neutron Laue diffraction. Our data establish the existence of a reentrant magnetoelectric phase between 19 T and 21 T. We show that a magnetized version of the zero field commensurate structure explains the magnetoelectric response quantitatively. The stability of this structure suggests a field-dependent spin anisotropy. Above 21 T, amagnetoelectrically inactive, short-wavelength incommensurate structure is identified. Our results demonstrate the combination of pulsed fields with epithermal neutron Laue diffraction as a powerful method to probe even complex phase diagrams in strong magnetic fields.
Formation Mechanism of Maghemite Nanoflowers Synthesized by a Polyol-Mediated Process

Magnetic nanoparticles are being developed as structural and functional materials for use in diverse areas, including biomedical applications. Here, we report the synthesis of maghemite (γ-Fe₂O₃) nanoparticles with distinct morphologies: single-core and multicore, including hollow spheres and nanoflowers, prepared by the polyol process. We have used sodium acetate to control the nucleation and assembly process to obtain the different particle morphologies. Moreover, from samples obtained at different time steps during the synthesis, we have elucidated the formation mechanism of the nanoflowers: the initial phases of the reaction present a lepidocrocite (γ-FeOOH) structure, which suffers a fast dehydroxylation, transforming to an intermediate “undescribed” phase, possibly a partly dehydroxylated lepidocrocite, which after some incubation time evolves to maghemite nanoflowers. Once the nanoflowers have been formed, a crystallization process takes place, where the γ-Fe₂O₃ crystallites within the nanoflowers grow in size (from ~11 to 23 nm), but the particle size of the flower remains essentially unchanged (~60 nm). Samples with different morphologies were coated with citric acid and their heating capacity in an alternating magnetic field was evaluated. We observe that nanoflowers with large cores (23 nm, controlled by annealing) densely packed (tuned by low NaAc concentration) offer 5 times enhanced heating capacity compared to that of the nanoflowers with smaller core sizes (15 nm), 4 times enhanced heating effect compared to that of the hollow spheres, and 1.5 times enhanced heating effect compared to that of single-
core nanoparticles (36 nm) used in this work.

**General information**

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Organisations: Neutrons and X-rays for Materials Physics, Department of Physics, CSIC, Universidad de Zaragoza
Authors: Gavilán, H. (Ekstern), Sánchez, E. H. (Ekstern), Brollo, M. E. F. (Ekstern), Asín, L. (Ekstern), Moerner, K. K. (Intern), Frandsen, C. (Intern), Lázaro, F. J. (Ekstern), Serna, C. J. (Ekstern), Veintemillas-Verdaguer, S. (Ekstern), Morales, M. P. (Ekstern), Gutiérrez, L. (Ekstern)
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**From concept to in vivo testing: Microcontainers for oral drug delivery**

This work explores the potential of polymeric micrometer sized devices (microcontainers) as oral drug delivery systems (DDS). Arrays of detachable microcontainers (D-MCs) were fabricated on a sacrificial layer to improve the handling and facilitate the collection of individual D-MCs. A model drug, ketoprofen, was loaded into the microcontainers using supercritical CO2 impregnation, followed by deposition of an enteric coating to protect the drug from the harsh gastric environment and to provide a fast release in the intestine. In vitro, in vivo and ex vivo studies were performed to assess the viability of the D-MCs as oral DDS. D-MCs improved the relative oral bioavailability by 180% within 4h, and increased the absorption rate by 2.4 times compared to the control. This work represents a significant step forward in the translation of these devices from laboratory to clinic.

**General information**

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Glycine buffered synthesis of layered iron(II)-iron(III) hydroxides (green rusts)

Layered Fe(II)-Fe(III) hydroxides (green rusts, GRs) are efficient reducing agents against oxidizing contaminants such as chromate, nitrate, selenite, and nitroaromatic compounds and chlorinated solvents. In this study, we adopted a buffered precipitation approach where glycine (GLY) was used in the synthesis of sulfate-interlayered GR (GRSO4) by aerial oxidation of Fe(II) or co-precipitation by adding Fe(III) salt to an aqueous solution of Fe(II) at constant pH. In both the oxidation and the co-precipitation methods pure crystalline GRSO4 was precipitated in the presence of 70mM GLY (pH 8.0), whereas in the absence of GLY, synthesis failed under similar conditions. Glycine functions as both a pH buffer and a ligand; Fe(II)-GLY complexes serve as a source of base (Fe(II)-GLY+H2O→Fe(II)+H-GLY+OH(-)) during GR formation, supplying about 45% of the total base required for the synthesis. The GLY buffer decreases pH fluctuations during base addition and hence allows for fast GRSO4 precipitation, minimizing byproduct formation. The use of other pH buffers [4-(2-hydroxyethyl)piperazine-1-ethanesulfonic acid and 2-amino-2-(hydroxymethyl)-1,3-propanediol] was also tested but failed. Mössbauer spectroscopy, X-ray diffraction, Fourier transform infrared, transmission electron microscopy, and Fe(II) measurements confirmed the purity, stoichiometry, and pyroaurite-type structure of the obtained GRSO4. The formula of
GRSO₄ was found to be Fe(II)₄.08Fe(III)₁.₉₈(OH)₁₁.₆(SO₄)₁.₀₀, and the tabular GR crystals had a lateral size of 100-500nm and a thickness of about 40nm. Upscaling of the synthesis by either 25 times in volume or 20 times in Fe(II) concentration resulted in pure GRSO₄ products. Compared with the conventional unbuffered GRSO₄ synthesis method, the present method can provide pure products with a controllable, fast, and low-cost process.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Aarhus University
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BFI (2014): BFI-level 1
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BFI (2011): BFI-level 1
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Scopus rating (2008): SJR 1.144 SNIP 1.335
Scopus rating (2007): SJR 1.026 SNIP 1.369
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Scopus rating (2006): SJR 0.992 SNIP 1.366
Web of Science (2006): Indexed yes
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Grain interaction mechanisms leading to intragranular orientation spread in tensile deformed bulk grains of interstitial-free steel

The spatially resolved intragranular orientation spread in two representative bulk grains of interstitial-free steel deformed to 9% tension has been investigated. A three-dimensional X-ray diffraction microscopy experiment revealed that the two similarly oriented grains are both embedded in local environments representing the bulk texture, yet their deformation-induced rotations are very different. The ALAMEL model is employed to analyse the grain interaction mechanisms. Predictions of this model qualitatively agree with the directionality and magnitude of the experimental orientation spread. However, quantitative agreement requires fine-tuning of the boundary conditions. The majority of the modelled slip is accounted for by four slip systems also predicted to be active by the classical Taylor model in uniaxial tension, and most of the orientation spread along the grain boundaries is caused by relative variations in the activities of these. Although limited to two grains, the findings prove that shear at the grain boundaries as accounted for by the ALAMEL model is a dominant grain interaction mechanism.

General information
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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
Authors: Winther, G. (Intern), Wright, J. P. (Ekstern), Schmidt, S. (Intern), Oddershede, J. (Intern)
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Improved orientation sampling for indexing diffraction patterns of polycrystalline materials

Orientation mapping is a widely used technique for revealing the microstructure of a polycrystalline sample. The crystalline orientation at each point in the sample is determined by analysis of the diffraction pattern, a process known as pattern indexing. A recent development in pattern indexing is the use of a brute-force approach, whereby diffraction patterns are simulated for a large number of crystalline orientations and compared against the experimentally observed diffraction pattern in order to determine the most likely orientation. Whilst this method can robustly identify orientations in the presence of noise, it has very high computational requirements. In this article, the computational burden is reduced by developing a method for nearly optimal sampling of orientations. By using the quaternion representation of orientations, it is shown that the optimal sampling problem is equivalent to that of optimally distributing points on a four-dimensional sphere. In doing so, the number of orientation samples needed to achieve a desired indexing accuracy is significantly reduced. Orientation sets at a range of sizes are generated in this way for all Laue groups and are made available online for easy use.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Neutrons and X-rays for Materials Physics
Authors: Larsen, P. M. (Intern), Schmidt, S. (Intern)
Iron oxide nanoparticles are widely prevalent in our aqueous environment (e.g., streams, seawater, hydrothermal vents). Their aggregation and crystal growth depend on their chemical surroundings, for instance just a change in pH or salt concentration can greatly affect this. In turn this influences their properties, mobility, fate, and environmental impact. We studied the growth of α-Fe₂O₃ (hematite), starting from 8 nm hematite particles in weakly acidic (HNO₃) aqueous suspension with different states of particle aggregation, using salt (NaCl and NaH₂PO₄) to control their initial aggregation state. The samples were then subject to hydrothermal treatment at 100-140 degrees C. We followed the development in aggregation state and particle size by dynamic light scattering, X-ray diffraction, small angle neutron scattering and transmission electron microscopy, and the magnetic properties by Mossbauer spectroscopy. The addition of NaCl and NaH₂PO₄ both led to aggregation, but NaCl led to linear chains of hematite nanoparticles (oriented parallel to their hexagonal c-axis), such that the crystalline lattice planes of neighboring hematite particles were aligned. However, despite this oriented alignment, the particles did not merge and coalesce. Rather they remained stable as mesocrystals until heat-treated. In turn, the addition of NaCl significantly increases the rate of growth during hydrothermal treatment, probably because the nanoparticles, due to the chain formation, are already aligned and in close proximity. With hydrothermal treatment, the magnetic properties of the particles transform from those characteristic of small (aggregated) hematite nanoparticles to those of particles with more bulk-like properties such as Morin transition and suppression of superparamagnetic relaxation, in correspondence with the growth of particle size.
In-Situ X-ray Tomography Study of Cement Exposed to CO₂ Saturated Brine

For successful CO₂ storage in underground reservoirs, the potential problem of CO₂ leakage needs to be addressed. A profoundly improved understanding of the behavior of fractured cement under realistic subsurface conditions including elevated temperature, high pressure and the presence of CO₂ saturated brine is required. Here, we report in situ X-ray micro computed tomography (μ-CT) studies visualizing the microstructural changes upon exposure of cured Portland cement with an artificially engineered leakage path (cavity) to CO₂ saturated brine at high pressure. Carbonation of the bulk cement, self-healing of the leakage path in the cement specimen, and leaching of CaCO₃ were thus directly observed. The precipitation of CaCO₃, which is of key importance as a possible healing mechanism of fractured cement, was found to be enhanced in confined regions having limited access to CO₂. For the first time, the growth kinetics of CaCO₃ under more realistic well conditions have thus been estimated quantitatively. Combining the μ-CT observations with scanning electron microscopy resulted in a detailed understanding of the processes involved in the carbonation of cement.
Ligand manipulation of charge transfer excited state relaxation and spin crossover in \([\text{Fe}(2,2^\prime\text{-bipyridine})_2(\text{CN})_2]^{2-}\)

We have used femtosecond resolution UV-visible and Kβ x-ray emission spectroscopy to characterize the electronic excited state dynamics of \([\text{Fe}(\text{bpy})_2(\text{CN})_2]^{2-}\), where bpy=2,2′-bipyridine, initiated by metal-to-ligand charge transfer (MLCT) excitation. The excited-state absorption in the transient UV-visible spectra, associated with the 2,2′-bipyridine radical anion, provides a robust marker for the MLCT excited state, while the transient Kβ x-ray emission spectra provide a clear measure of intermediate and high spin metal-centered excited states. From these measurements, we conclude that the MLCT state of \([\text{Fe}(\text{bpy})_2(\text{CN})_2]^{2-}\) undergoes ultrafast spin crossover to a metal-centered quintet excited state through a short lived metal-centered triplet transient species. These measurements of \([\text{Fe}(\text{bpy})_2(\text{CN})_2]^{2-}\) complement prior measurement performed on \([\text{Fe}(\text{bpy})_3]^{2+}\) and \([\text{Fe}(\text{bpy})(\text{CN})_4]^{2-}\) in dimethylsulfoxide solution and help complete the chemical series \([\text{Fe}(\text{bpy})(\text{CN})_6]^{2N-4}\), where \(N = 1\)–3. The measurements confirm that simple ligand modifications can significantly change the relaxation pathways and excited state lifetimes and support the further investigation of light harvesting and photocatalytic applications of 3d transition metal complexes.
Magnetic dipolar ordering and hysteresis of geometrically defined nanoparticle clusters

Magnetic nanoparticle clusters have several biomedical and engineering applications, and revealing the basic interplay between particle configuration and magnetic properties is important for tuning the clusters for specific uses. Here, we consider the nanoparticles as macrospins and use computer simulations to determine their magnetic configuration when placed at the vertices of various polyhedra. We find that magnetic dipoles of equal magnitude arrange in flux-closed vortices on a layer basis, giving the structures a null remanent magnetic moment. Assigning a toroidal moment to each layer, we find that the geometrical arrangement, i.e., “triangular packing” vs. “square packing,” of the moments in the adjacent layer determines whether the flux-closed layers are ferrotoroidal (co-rotating vortices) or antiferrotoroidal (counter-rotating vortices). Interestingly, upon adding a single magnetic moment at the center of the polyhedra, the central moment relaxes along one of the principal axes and induces partial alignment of the surrounding moments. The resulting net moment is up to nearly four times that of the single moment added. Furthermore, we model quasi-static hysteresis loops for structures with and without a central moment. We find that a central moment ensures an opening of the hysteresis loop, and the resultant loop areas are typically many-fold larger compared to the same structure without a central moment.
Magnetic order, hysteresis, and phase coexistence in magnetoelectric LiCoPO$_4$

The magnetic phase diagram of magnetoelectric LiCoPO$_4$ is established using neutron diffraction and magnetometry in fields up to 25.9 T applied along the crystallographic b axis. For fields greater than 11.9 T, the magnetic unit cell triples in size with propagation vector $Q = (0, 1/3, 0)$. A magnetized elliptic cycloid is formed with spins in the (b, c) plane and the major axis oriented along b. Such a structure allows for the magnetoelectric effect with an electric polarization along c induced by magnetic fields applied along b. Intriguingly, additional ordering vectors $Q \approx (0, 1/4, 0)$ and $Q \approx (0, 1/2, 0)$ appear for increasing fields in the hysteresis region below the transition field. Traces of this behavior are also observed in the magnetization. A simple model based on a mean-field approach is proposed to explain these additional ordering vectors. In the field interval 20.5-21.0 T, the propagation vector $Q = (0, 1/3, 0)$ remains but the spins orient differently compared to the cycloid phase. Above 21.0 T and up until saturation, a commensurate magnetic structure exists with a ferromagnetic component along b and an antiferromagnetic component along c.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technical University of Denmark, Iowa State University, Helmholtz-Zentrum Berlin für Materialien und Energie, Université Grenoble Alpes, Paul Scherrer Institut, University of Copenhagen
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Scopus rating (2010): SJR 3.417 SNIP 1.451
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution

Developing light-harvesting and photocatalytic molecules made with iron could provide a cost effective, scalable, and environmentally benign path for solar energy conversion. To date these developments have been limited by the sub-picosecond metal-to-ligand charge transfer (MLCT) electronic excited state lifetime of iron based complexes due to spin crossover—the extremely fast intersystem crossing and internal conversion to high spin metal-centered excited states. We revitalize a 30 year old synthetic strategy for extending the MLCT excited state lifetimes of iron complexes by making mixed ligand iron complexes with four cyanide (CN⁻) ligands and one 2,2'-bipyridine (bpy) ligand. This enables MLCT excited state and metal-centered excited state energies to be manipulated with partial independence and provides a path to suppressing spin crossover. We have combined X-ray Free-Electron Laser (XFEL) Kβ hard X-ray fluorescence spectroscopy with femtosecond time-resolved UV-visible absorption spectroscopy to characterize the electronic excited state dynamics initiated by MLCT excitation of [Fe(CN)₄(bpy)]²⁻. The two experimental techniques are highly complementary; the time-resolved UV-visible measurement probes allowed electronic transitions between valence states making it sensitive to ligand-centered electronic states such as MLCT states, whereas the Kβ fluorescence spectroscopy provides a sensitive measure of changes in the Fe spin state characteristic of metal-centered excited states. We conclude that the MLCT excited state of [Fe(CN)₄(bpy)]²⁻ decays with roughly a 20 ps lifetime without undergoing spin crossover, exceeding the MLCT excited state lifetime of [Fe(2,2'-bipyridine)₃]²⁺ by more than two orders of magnitude.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Stanford University, Lund University, SLAC National Accelerator Laboratory, Max Planck Institute for Biophysical Chemistry
Measured resolved shear stresses and Bishop-Hill stress states in individual grains of austenitic stainless steel

The full three-dimensional stress state of 172 individual bulk grains in austenitic stainless steel 316L at 0.1 and 1% sample elongation has been determined with sufficient accuracy to allow comparison with the theoretical Bishop-Hill stress states for plastically deforming grains as well as calculation of the resolved shear stresses on the individual slip systems. At 0.1%, the resolved shear stresses exhibit quite large variations between grains of similar orientation. When averaging over similarly oriented grains, the resolved shear stresses correspond to the Schmid factors for uniaxial tension. At 1%, only about half of the grains were close to a Bishop-Hill stress state. The stress state of the other half of the grains was closer to the applied uniaxial stress, in between Bishop-Hill states, or in some cases none of these. The orientation dependence of the assigned stress states deviate somewhat from the theoretical expectation. These deviations are found to originate from a larger tensile stress component than in the theoretical Bishop-Hill stress states and to be associated also with deviations from axisymmetric plastic strain. This conclusion was supported by finite-element crystal plasticity simulations.

General information
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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, University of Illinois at Urbana-Champaign, Cornell High Energy Synchrotron Source, Air Force Research Laboratory
Microfabrication of gratings for X-ray phase contrast imaging

General information
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Organisations: DTU Danchip, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Silvestre, C. (Intern), Hemmingsen, J. H. (Intern), Christensen, E. D. (Forskerdatabase), Kehres, J. (Intern), Hansen, O. (Intern)
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Modeling surface imperfections in thin films and nanostructured surfaces

Accurate scatterometry and ellipsometry characterization of non-perfect thin films and nanostructured surfaces are challenging. Imperfections like surface roughness make the associated modelling and inverse problem solution difficult due to the lack of knowledge about the imperfection on the surface. Combining measurement data from several instruments increases the knowledge of non-perfect surfaces. In this paper we investigate how to incorporate this knowledge of surface imperfection into inverse methods used in scatterometry and ellipsometry using the Rigorous Coupled Wave Analysis. Three classes of imperfections are examined. The imperfections are introduced as periodic structures with a super cell periods ten times larger than the simple grating period. Two classes of imperfections concern the grating and one class concern the substrate. It is shown that imperfections of a few nanometers can severely change the reflective response on silicon gratings. Inverse scatterometry analyses of gratings with imperfection using simulated data with white noise have been performed. The results show that scatterometry is a robust technology that is able to characterize grating imperfections provided that the imperfection class is known.

General information
Molecular scale structure and dynamics at an ionic liquid/electrode interface

After a century of research, the potential-dependent ion distribution at electrode/electrolyte interfaces is still under debate. In particular for solvent-free electrolytes such as room-temperature ionic liquids, classical theories for the electrical double layer are not applicable. Using a combination of in situ high-energy X-ray reflectivity and impedance spectroscopy measurements, we determined this distribution with sub-molecular resolution. We find oscillatory charge density profiles consisting of alternating anion- and cation-enriched layers at both cathodic and anodic potentials. This structure is shown to arise from the same ion-ion correlations dominating the liquid bulk structure. The relaxation dynamics of the interfacial structure upon charging/discharging were studied by impedance spectroscopy and time resolved X-ray reflectivity experiments with sub-millisecond resolution. The analysis revealed three relaxation processes of vastly different characteristic time scales: a 2 ms scale interface-normal ion transport, a 100 ms scale molecular reorientation, and a minute scale lateral ordering within the first layer.
Monte Carlo Particle Lists: MCPL
A binary format with lists of particle state information, for interchanging particles between various Monte Carlo simulation applications, is presented. Portable C code for file manipulation is made available to the scientific community, along with converters and plugins for several popular simulation packages.

Program summary:
Program Title: MCPL
Program Files doi: http://dx.doi.org/10.17632/cby92vsv5g.1
Licensing provisions: CC0 for core MCPL, see LICENSE file for details. Programming language: C and C++
External routines/libraries: Geant4, MCNP, McStas, McXtrace
Nature of problem: Saving particle states in Monte Carlo simulations, for interchange between simulation packages or for reuse within a single package. Solution method: Binary interchange format with associated code written in portable C along with tools and interfaces for relevant simulation packages.

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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB
MultiFLEXX - The new multi-analyzer at the cold triple-axis spectrometer FLEXX

The first experimental characterization of a multiple energy analysis wide angle backend for a cold triple-axis spectrometer is reported. The multi-analyzer module MultiFLEXX employs 155 detection channels which simultaneously probe an extensive range in wavevector and energy transfer. Successful mapping of magnetic excitations in MnF$_2$ and Ho demonstrate order of magnitude gains in data collection efficiency using this novel type backend. MultiFLEXX is competitive to standard triple-axis spectroscopy in terms of energy resolution and signal-to-noise ratio. A minority of the detector channels is affected by spurious signals inherent to this multiplexing concept. The characteristic signature of these spurious signals easily allows for their discrimination. The instrument concept focuses on detection efficiency in the horizontal scattering plane which makes it an ideal technique for fast mapping and parametric studies including extreme sample environment.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Helmholtz–Zentrum Berlin für Materialien und Energie, Technische Universitat Dresden, China Institute of Atomic Energy
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
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Multispectral x-ray CT: multivariate statistical analysis for efficient reconstruction

Recent developments in multispectral X-ray detectors allow for an efficient identification of materials based on their chemical composition. This has a range of applications including security inspection, which is our motivation. In this paper, we analyze data from a tomographic setup employing the MultiX detector, that records projection data in 128 energy bins covering the range from 20 to 160 keV. Obtaining all information from this data requires reconstructing 128 tomograms, which is computationally expensive. Instead, we propose to reduce the dimensionality of projection data prior to reconstruction and reconstruct from the reduced data. We analyze three linear methods for dimensionality reduction using a dataset with 37 equally-spaced projection angles. Four bottles with different materials are recorded for which we are able to obtain similar discrimination of their content using a very reduced subset of tomograms compared to the 128 tomograms that would otherwise be needed without dimensionality reduction.

Off-axis spin orientation in goethite nanoparticles

Neutron diffraction is a powerful technique for determining the magnetic structure of antiferromagnetic materials. However, for some of these, determining the detailed magnetic structure remains a challenge. In goethite (α-FeOOH) the antiferromagnetic unit cell coincides with the chemical unit cell and, consequently, nuclear and magnetic diffraction peaks occur at the same positions. Analysis of diffraction data from goethite is further complicated by finite-size peak broadening, resulting from goethite commonly occurring in nanocrystalline form. For these reasons, determining the magnetic structure of goethite has been challenging, and few detailed studies have been published. Even today, not all aspects of the magnetic structure are well established. Here, we investigate the magnetic structure of three samples of goethite nanoparticles with polarized neutron powder diffraction (xyz-polarization analysis). Two samples consist of acicular goethite particles that are approximately 40 nm long and with different thicknesses, and one sample consists of pseudospherical particles with a diameter of approximately 5 nm. The larger particles consist of several crystallites whereas the 5-nm particles are mostly single crystalline. The polarization analysis enables us to separate magnetic scattering from nuclear and spin-incoherent scattering, resulting in data that can readily be analyzed. For the two samples with the larger particle size, we find nuclear correlation lengths in the [100] direction that are approximately 3 nm longer than the magnetic correlation lengths, indicating a magnetically disordered layer perpendicular to the antiferromagnetic modulation direction. We find no evidence of a magnetically disordered surface layer in the 5-nm particles. We find the magnetic structure to be antiferromagnetic but, in contrast to most previous studies, we find the spin orientation in all three samples to make an angle of 28-30° with respect to the crystallographic b axis.
On the 'centre of gravity' method for measuring the composition of magnetite/maghemite mixtures, or the stoichiometry of magnetite-maghemite solid solutions, via $^{57}$Fe Mössbauer spectroscopy

We evaluate the application of $^{57}$Fe Mössbauer spectroscopy to the determination of the composition of magnetite ($\text{Fe}_3\text{O}_4$)/maghemite ($\gamma\text{-Fe}_2\text{O}_3$) mixtures and the stoichiometry of magnetite-maghemite solid solutions. In particular, we consider a recently proposed model-independent method which does not rely on a priori assumptions regarding the nature of the sample, other than that it is free of other Fe-containing phases. In it a single parameter, $\bar{\delta}_R T$, the ‘centre of gravity’, or area weighted mean isomer shift at room temperature, $T = 295 \pm 5$ K-is extracted by curve-fitting a sample's Mössbauer spectrum, and is correlated to the sample's composition or stoichiometry. We present data on high-purity magnetite and maghemite powders, and mixtures thereof, as well as comparison literature data from nanoparticulate mixtures and solid solutions, to show that a linear correlation exists between $\bar{\delta}_R T$ and the numerical proportion of Fe atoms in the magnetite environment: $\alpha = \frac{\text{Fe}^{\text{magnetite}}}{\text{Fe}^{\text{total}}} = \frac{(\bar{\delta}_R T - \bar{\delta}_o)}{m}$, where $\bar{\delta}_o = 0.3206 \pm 0.0022$ mm s$^{-1}$ and $m = 0.2135 \pm 0.0076$ mm s$^{-1}$. We also present equations to relate $\alpha$ to the weight percentage $w$ of magnetite in mixed phases, and the magnetite stoichiometry $x = \text{Fe}^{2+}/\text{Fe}^{3+}$ in solid solutions. The analytical method is generally applicable, but is most accurate when the absorption profiles are sharp; in some samples this may require spectra to be recorded at reduced temperatures. We consider such cases and provide equations to relate $\delta(T)$ to the corresponding $\alpha$ value.

General information

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Scopus rating (2015): SJR 0.693 SNIP 1.046 CiteScore 2.1
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.069 SNIP 1.383 CiteScore 2.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
On the elusive crystal structure of expanded austenite

No consistent structural description exists for expanded austenite that accurately accounts for the hkl-dependent peak shifts and broadening observed in diffraction experiments. The best available description for homogeneous samples is a face-centered cubic lattice with stacking faults. Here Debye simulations of stacking fault effects were compared to experimental data for macro-stress free homogeneous expanded austenite to show that a faulted structure cannot explain the observed peak displacement anomalies. Instead it is argued that the shifts are the combined result of elastic and plastic anisotropy leading to (strongly) non-linear hkl-dependent elastic behavior during composition-induced plastic deformation on synthesis of expanded austenite.
Herein we present surface sensitive operando XAS L-edge measurements on IrO$_x$/RuO$_x$ thin films as well as mass-selected RuO$_x$ and Ru nanoparticles. We observed shifts of the white line XAS peak toward higher energies with applied electrochemical potential. Apart from the case of the metallic Ru nanoparticles, the observed potential dependencies were purely core-level shifts caused by a change in oxidation state, which indicates no structural changes. These findings can be explained by different binding energies of oxygenated species on the surface of IrO$_x$ and RuO$_x$. Simulated XAS spectra show that the average Ir oxidation state change is strongly affected by the coverage of atomic O. The observed shifts in oxidation state suggest that the surface has a high coverage of O at potentials just below the potential where oxygen evolution is exergonic in free energy. This observation is consistent with the notion that the metal-oxygen bond is stronger than ideal.
Optical simulations for design, alignment, and performance prediction of silicon pore optics for the ATHENA x-ray telescope

The ATHENA X-ray observatory is a large-class ESA approved mission, with launch scheduled in 2028. The technology of silicon pore optics (SPO) was selected as baseline to assemble ATHENA’s optic with hundreds of mirror modules, obtained by stacking wedged and ribbed silicon wafer plates onto silicon mandrels to form the Wolter-I configuration. In the current configuration, the optical assembly has a 3 m diameter and a 2 m2 effective area at 1 keV, with a required angular resolution of 5 arcsec. The angular resolution that can be achieved is chiefly the combination of 1) the focal spot size determined by the pore diffraction, 2) the focus degradation caused by surface and profile errors, 3) the aberrations introduced by the misalignments between primary and secondary segments, 4) imperfections in the co-focality of the mirror modules in the optical assembly. A detailed simulation of these aspects is required in order to assess the fabrication and alignment tolerances; moreover, the achievable effective area and angular resolution depend on the mirror module design. Therefore, guaranteeing these optical performances requires: a fast design tool to find the most performing solution in terms of mirror module geometry and population, and an accurate point spread function simulation from local metrology and positioning information. In this paper, we present the results of simulations in the framework of ESA-
financed projects (SIMPOSiuM, ASPHEA, SPIRIT), in preparation of the ATHENA X-ray telescope, analyzing the mentioned points: 1) we deal with a detailed description of diffractive effects in an SPO mirror module, 2) we show ray-tracing results including surface and profile defects of the reflective surfaces, 3) we assess the effective area and angular resolution degradation caused by alignment errors between SPO mirror module’s segments, and 4) we simulate the effects of co-focality errors in X-rays and in the UV optical bench used to study the mirror module alignment and integration.

General information
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Organisations: National Space Institute, Astrophysics and Atmospheric Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Cosine Science and Computing B.V., Technical University of Denmark, INAF - Brera Astronomical Observatory, ESTEC, Media Lario S.r.l., Politecnico di Milano
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Porosity and density measurements of sodium acetate trihydrate for thermal energy storage
Sodium acetate trihydrate (SAT) can be used as phase change material in latent heat storage with or without utilizing supercooling. The change of density between liquid to solid state leads to formation of cavities inside the bulk SAT during solidification. Samples of SAT which had solidified from supercooled state at ambient temperature and samples which had solidified with a minimal degree supercooled were investigated. The temperature dependent densities of liquid and the two types of solid SAT were measured with a density meter and a thermomechanical analyzer. The cavities formed inside samples of solid SAT, which had solidified after a high or minimal degree of supercooling, were investigated by X-ray scanning and computer tomography. The apparent density of solid SAT depended on whether it solidified from a supercooled state or not. A sample which solidified from a supercooled liquid contained 15% cavities and had a density of 1.26 g/cm³ at 25 °C. SAT which had solidified with minimal supercooling contained 9% cavities and had a density of 1.34 g/cm³ at 25 °C. The apparent densities of the solid SAT samples were significant lower than the value of solid SAT reported in literature of 1.45 g/cm³. The density of liquid and supercooled SAT with extra water was also determined at different temperatures.

General information
State: Accepted/In press
Organisations: Department of Civil Engineering, Section for Building Energy, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, University of Zaragoza, Technical University of Denmark, Graz University of Technology
Publication date: 2017
Main Research Area: Technical/natural sciences
Sodium acetate trihydrate, Density, Phase change material, X-ray tomography, Thermal energy storage, Cavity
Powder embossing method for selective loading of polymeric microcontainers with drug formulation

The present study introduces powder embossing as a novel method to enhance loading of polymeric microcontainers with drug. With current loading approaches, it is not possible to handle pure powder drug in a scalable, homogenous and reproducible manner. In this work, we demonstrate simultaneous loading of 625 microcontainers with powder formulation. This is achieved in a single step by aligning a shadow mask prepared by micro-milling to an array of microcontainers in order to limit drug deposition to the container cavities with diameters of 220 μm. A pressure of 8.9 MPa is applied by a bonding press and thereby the desired powder is embossed into the container cavities. Powder in the form of pure drug, lipid-based microparticles, and pure polymer was successfully loaded with minimal residues in between the microcontainers and with 100% loaded cavities demonstrating the versatility of the method. The current work is thus contributing to the loading of powder formulations into microscale drug delivery systems such as microcontainers in a facile and reproducible manner.

General information
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Organisations: Department of Micro- and Nanotechnology, Department of Physics, Neutrons and X-rays for Materials Physics, Nanoprobes, Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.69 SJR 0.606 SNIP 0.999
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.533 SNIP 0.856 CiteScore 1.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.592 SNIP 0.897 CiteScore 1.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.602 SNIP 1.001 CiteScore 1.45
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.745 SNIP 0.983 CiteScore 1.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.818 SNIP 1.169 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.946 SNIP 1.119
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.847 SNIP 1.127
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scene reassembly after multimodal digitization and pipeline evaluation using photorealistic rendering

Transparent objects require acquisition modalities that are very different from the ones used for objects with more diffuse reflectance properties. Digitizing a scene where objects must be acquired with different modalities requires scene reassembly after reconstruction of the object surfaces. This reassembly of a scene that was picked apart for scanning seems unexplored. We contribute with a multimodal digitization pipeline for scenes that require this step of reassembly. Our pipeline includes measurement of bidirectional reflectance distribution functions and high dynamic range imaging of the lighting environment. This enables pixelwise comparison of photographs of the real scene with renderings of the digital version of the scene. Such quantitative evaluation is useful for verifying acquired material appearance and reconstructed surface geometry, which is an important aspect of digital content creation. It is also useful for identifying and improving issues in the different steps of the pipeline. In this work, we use it to improve reconstruction, apply analysis by synthesis to estimate optical properties, and to develop our method for scene reassembly.

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BFI (2018): BFI-level 1
Simulating and optimizing compound refractive lens-based X-ray microscopes

A comprehensive optical description of compound refractive lenses (CRLs) in condensing and full-field X-ray microscopy applications is presented. The formalism extends ray-transfer matrix analysis by accounting for X-ray attenuation by the lens material. Closed analytical expressions for critical imaging parameters such as numerical aperture, spatial acceptance (vignetting), chromatic aberration and focal length are provided for both thin- and thick-lens imaging geometries. These expressions show that the numerical aperture will be maximized and chromatic aberration will be minimized at the thick-lens limit. This limit may be satisfied by a range of CRL geometries, suggesting alternative approaches to improving the resolution and efficiency of CRLs and X-ray microscopes.

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Ratings:
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.593 SNIP 1.578
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.161 SNIP 1.396 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.505 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.473 SNIP 1.687 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.558 SNIP 1.273 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.503 SNIP 1.424 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.618 SNIP 1.479
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.496 SNIP 1.373
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.938 SNIP 1.637
SiO$_2$ Glass Density to Lower-Mantle Pressures

The convection or settling of matter in the deep Earth's interior is mostly constrained by density variations between the different reservoirs. Knowledge of the density contrast between solid and molten silicates is thus of prime importance to understand and model the dynamic behavior of the past and present Earth. SiO$_2$ is the main constituent of Earth's mantle and is the reference model system for the behavior of silicate melts at high pressure. Here, we apply our recently developed x-ray absorption technique to the density of SiO$_2$ glass up to 110 GPa, doubling the pressure range for such measurements. Our density data validate recent molecular dynamics simulations and are in good agreement with previous experimental studies conducted at lower pressure. Silica glass rapidly densifies up to 40 GPa, but the density trend then flattens to become asymptotic to the density of SiO$_2$ minerals above 60 GPa. The density data present two discontinuities at similar to 17 and similar to 60 GPa that can be related to a silicon coordination increase from 4 to a mixed 5/6 coordination and from 5/6 to sixfold, respectively. SiO$_2$ glass becomes denser than MgSiO$_3$ glass at similar to 40 GPa, and its density becomes identical to that of MgSiO$_3$ glass above 80 GPa. Our results on SiO$_2$ glass may suggest that a variation of SiO$_2$ content in a basaltic or pyrolytic melt with pressure has at most a minor effect on the final melt density, and iron partitioning between the melts and residual solids is the predominant factor that controls melt buoyancy in the lowermost mantle.
Spin excitations and quantum criticality in the quasi-one-dimensional Ising-like ferromagnet CoCl₂·2D₂O in a transverse field

We present experimental evidence for a quantum phase transition in the easy-axis $S = 3/2$ anisotropic quasi-one-dimensional ferromagnet CoCl₂·2D₂O in a transverse field. Elastic neutron scattering shows that the magnetic order parameter vanishes at a transverse critical field $\mu_0 H_c = 16.05(4)$ T, while inelastic neutron scattering shows that the gap in the magnetic excitation spectrum vanishes at the same field value, and reopens for $H > H_c$. The field dependence of the order parameter and the gap are well described by critical exponents $\beta = 0.45 \pm 0.09$ and $z \nu$ close to $1/2$, implying that the quantum phase transition in CoCl₂·2D₂O differs significantly from the textbook version of a $S = 1/2$ Ising chain in a transverse field. We attribute the difference to weak but finite three-dimensionality of the magnetic interactions.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, ESS Data Management & Software Center, Oak Ridge National Laboratory, Ecole Polytechnique Federale de Lausanne (EPFL)
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Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Spin orientation in solid solution hematite-ilmenite

The spin orientation in synthetic hematite-ilmenite samples and in a sample of natural hematite was studied from room temperature to above the antiferromagnetic-paramagnetic phase transition (the Néel temperature; TN = 600–950 K) by neutron powder diffraction and at room temperature by Mössbauer spectroscopy. The usually assumed magnetic structure of hematite within this temperature range is antiferromagnetic with the spins confined to the basal plane of the hexagonal structure; however, an out-of-plane spin component is allowed by the symmetry of the system and has been observed in recent studies of synthetic hematite samples. We find the spins in the antiferromagnetic sublattices to be rotated out of the basal plane by an angle between 11(2)° and 22.7(5)° in both synthetic hematite-ilmenite samples and in the natural hematite sample. The spin angle remains tilted out of the basal plane in the entire temperature range below the Néel temperature and does not depend systematically on Ti-content. The results indicate that the out-of-plane spin component is an intrinsic feature of hematite itself, with an origin not yet fully understood, but consistent with group theory. This represents a major shift in understanding of one of the two main mineral systems responsible for rock magnetism.
Stability of charge-stripe ordered $\text{La}_{2-x}\text{Sr}_{x}\text{NiO}_{4+\delta}$ at one third doping

The stability of charge ordered phases is doping dependent, with different materials having particularly stable ordered phases. In the half filled charge ordered phases of the cuprates this occurs at one eighth doping, whereas in charge-stripe ordered $\text{La}_{2-x}\text{Sr}_{x}\text{NiO}_{4+\delta}$ there is enhanced stability at one third doping. In this paper we discuss the known details of the charge-stripe order in $\text{La}_{2-x}\text{Sr}_{x}\text{NiO}_{4+\delta}$, and how these properties lead to the one third doping stability.
Stochastic derivation and solution of simplified radiative transfer using the Fokker-Planck equation

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics, Technical University of Denmark
Authors: Karamehmedovic, M. (Intern), Chen, X. (Ekstern), Karamehmedovic, M. (Intern)
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Structural Analysis Algorithms for Nanomaterials
This thesis presents a reformulation of existing problems in materials science in terms of well-known methods from applied mathematics: graph theory, computational geometry, and mixed integer programming.

The centrosymmetry parameter is reformulated as a graph matching problem, and resolves the inconsistencies in the existing calculation methods as a consequence. By formulating the distance function of lattices as a bipartite graph matching problem, it is shown that the similarity between crystal lattices (root mean square distance, RMSD) can be calculated in polynomial time, which improves upon the existing factorial-time bound. This method is subsequently extended to two-dimensional monolayers.

A method is presented for the identification of ordered crystalline phases in molecular dynamics simulations. A robust classification is obtained by the use of template matching, also formulated as a bipartite matching problem on geometric graphs. This method is adapted for two-dimensional materials, in order that e.g. defect structures in polycrystalline graphene can be studied.

Matrix decompositions are used to develop a geometric lattice matching algorithm, which can exhaustively identify all low-strain interfaces. The stable, low-energy interfaces which are found as a result are intended for use in the design and construction of topological superconductors, which have important applications in quantum computing.

Cluster expansion models are used to find ground-state structures in gold-silver nanoparticles, which are used in a variety of catalysis processes. In addition to this concrete application, theoretical methods are developed for the optimal construction of cluster expansion models, the exact determination of ground states in a large model, and the exhaustive determination of all possible ground states in a small model.

Lastly, a method for nearly-optimal sampling of orientations is presented. Whilst this has many applications in science and engineering, the use-case described here is the indexing of diffraction patterns for experimental materials characterization. Significantly improved sampling is achieved by applying methods from computational geometry.

General information
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Authors: Larsen, P. M. (Intern), Schiøtz, J. (Intern), Schmidt, S. (Intern)
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Relations
Structural stability of naphthyl end-capped oligothiophenes in organic field-effect transistors measured by grazing-incidence X-ray diffraction in operando

We report on microstructural durability of 5,5′-bis(naphth-2-yl)-2,2′-bithiophene (NaT2) in organic field-effect transistors (OFETs) in operando monitored by grazing-incidence X-ray diffraction (GIXRD). NaT2 maintains its monoclinic bulk motif in operating OFETs with $a=20.31\pm0.06$ Å, $b=6.00\pm0.01$ Å, $c=8.17\pm0.04$ Å and $\beta=96.64\pm0.74^\circ$. Crystallites appear as a mosaic of single crystals reaching through the whole 50 nm thick active layer. The lattice parameters variation (<1%) falls within the statistical error of structure refinement when the OFET gate voltage is varied from 0 V to 40 V; or when the OFET is continuously cycled within this voltage interval over more than 10 h period. Within the first few cycles, both the hole mobility and threshold voltage are changing but then reach stable levels with an average mobility of $(3.25\pm0.04) \times 10^4$ cm²/Vs and an average threshold voltage of $13.6\pm0.2$ V, both varying less than 4% for the remainder of the 10 h period. This demonstrates crystalline stability of NaT2 in operating OFETs.
The Importance of Surface IrOx in Stabilizing RuO₂ for Oxygen Evolution

The high precious metal loading and high overpotential of the oxygen evolution reaction (OER) prevents the widespread utilization of polymer electrolyte membrane (PEM) water electrolyzers. Herein we explore the OER activity and stability in acidic electrolyte of a combined IrOx/RuO₂ system consisting of RuO₂ thin films with sub-monolayer (1, 2 and 4 Å) amounts of IrOx deposited on top. Operando extended X-ray absorption fine structure (EXAFS) on the Ir L-3 edge revealed a rutile type IrO₂ structure with some Ir sites occupied by Ru, IrOx being at the surface of the RuO₂ thin film. We monitor corrosion on IrO₅/RuO₂ thin films by combining electrochemical quartz crystal microbalance (EQCM) with inductively coupled mass spectrometry (ICP-MS). We elucidate the importance of sub-monolayer surface IrOx in minimizing Ru dissolution. Our work shows that we can tune the surface properties of active OER catalysts such as RuO₂, aiming to achieve higher electrocatalytic stability in PEM electrolyzers.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
The physical properties of polycrystalline materials depend on their microstructure, which is the nano- to centimeter scale arrangement of phases and defects in their interior. Such microstructure depends on the shape, crystallographic phase and orientation, and interfacing of the grains constituting the material. This article presents a new non-destructive 3D technique to study centimeter-sized bulk samples with a spatial resolution of hundred micrometers: time-of-flight three-dimensional neutron diffraction (ToF 3DND). Compared to existing analogous X-ray diffraction techniques, ToF 3DND enables studies of samples that can be both larger in size and made of heavier elements. Moreover, ToF 3DND facilitates the use of complicated sample environments. The basic ToF 3DND setup, utilizing an imaging detector with high spatial and temporal resolution, can easily be implemented at a time-of-flight neutron beamline. The technique was developed and tested with data collected at the Materials and Life Science Experimental Facility of the Japan Proton Accelerator Complex (J-PARC) for an iron sample. We successfully reconstructed the shape of 108 grains and developed an indexing procedure. The reconstruction algorithms have been validated by reconstructing two stacked Co-Ni-Ga single crystals, and by comparison with a grain map obtained by post-mortem electron backscatter diffraction (EBSD).
Towards identifying the active sites on RuO$_2$(110) in catalyzing oxygen evolution

While the surface atomic structure of RuO$_2$ has been well studied in ultra high vacuum, much less is known about the interaction between water and RuO$_2$ in aqueous solution. In this work, in situ surface X-ray scattering measurements combined with density functional theory (DFT) were used to determine the surface structural changes on single-crystal RuO$_2$(110) as a function of potential in acidic electrolyte. The redox peaks at 0.7, 1.1 and 1.4 V vs. reversible hydrogen electrode (RHE) could be attributed to surface transitions associated with the successive deprotonation of –H$_2$O on the coordinatively unsaturated Ru sites (CUS) and hydrogen adsorbed to the bridging oxygen sites. At potentials relevant to the oxygen evolution reaction (OER), an –OO species on the Ru CUS sites was detected, which was stabilized by a neighboring –OH group on the Ru CUS or bridge site. Combining potential-dependent surface structures with their energetics from DFT led to a new OER pathway, where the deprotonation of the –OH group used to stabilize –OO was
Ultrafast dynamics of two copper bis-phenanthroline complexes measured by x-ray transient absorption spectroscopy:

Ultrafast structural dynamics of the metal to ligand charge transfer (MLCT) states of two copper bis-phenanthroline complexes were captured by using x-ray transient absorption (XTA) spectroscopy at the Linac Coherent Light Source and further described by theoretical calculations. These complexes have the general formula [Cu(\text{R})_2]^+, where \text{R} = 2,9-dimethyl-1,10-phenanthroline (dmp) and 2,9-diphenyl-1,10-phenanthroline disulfonic acid disodium salt (dpps).
[Cu(I)(dmp)₂]⁺ has methyl groups at the 2,9 positions of phenanthroline (phen) and adopts a pseudo-tetrahedral geometry. In contrast, [Cu(I)(dpps)₂]⁺ possesses two bulky phenyl-sulfonate groups attached to each phen ligand that force the molecule to adopt a flattened tetrahedral geometry in the ground state. Previously, optical transient absorption (OTA) and synchrotron based XTA experiments with 100 ps time resolution have been employed to study the relationship between structural distortions and excited state relaxation pathways in the two complexes. However, the dynamics of the MLCT transition during the first few picoseconds after excitation in these complexes remained unclear because of limitations in element specificity in OTA and in the time resolution of synchrotron sources in XTA. In this experiment, the local coordination geometry and oxidation state of copper were probed with a temporal resolution of ~300 fs. Unexpectedly, the depletion of the Cu(I) signal due to the MLCT transition was found to be non-impulsive in the case of [Cu(I)(dpps)₂]⁺ with a time constant of 0.6 ps, while the Cu(I) depletion in [Cu(I)(dmp)₂]⁺ was instantaneous within the 300 fs instrument response time. The slower Cu(I) depletion kinetics in [Cu(I)(dpps)₂]⁺, previously unobserved in femtosecond OTA experiments, is likely due to intramolecular motions on the sub-picosecond time scale that could alter the localization of the transferred electron in the phen ligands.

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.22 SJR 0.616 SNIP 0.541
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.791 SNIP 0.806 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.121 SNIP 0.905 CiteScore 1.5
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.089 SNIP 0.943 CiteScore 1.62
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.18 SNIP 1.064 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.055 SNIP 0.931 CiteScore 1.7
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.099 SNIP 0.933
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.292 SNIP 1.073
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.478 SNIP 1.075
Web of Science (2008): Indexed yes
Ultra-low-angle boundary networks within recrystallizing grains

We present direct evidence of a network of well-defined ultra-low-angle boundaries in bulk recrystallizing grains of 99.5% pure aluminium (AA1050) by means of a new, three-dimensional X-ray mapping technique; dark-field X-ray microscopy. These boundaries separate lattice orientation differences on the order of 0.05° and thus subdivide the recrystallizing grain into 2–7 μm wide domains. During further annealing the orientation differences decrease and the overall structure become more uniform while the network remains. It is observed that the morphology of the grain boundaries surrounding the recrystallizing grains relate to the intragranular network and effects hereof on the boundary migration is discussed.

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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.347 SNIP 1.975 CiteScore 3.19
Poly(ethylene oxide) (PEO), thin films of different thicknesses (220, 450, and 1500 nm) and molecular masses (4000, 8000, and 20000 g/mol) have been fabricated by spin-coating of methanol solutions onto glass substrates. All these samples have been recrystallized from the melt using a directional thermal gradient technique. Millimeter-size domains with crystallites uniformly, oriented in the direction of the thermal gradient are observed. Furthermore, the crystallites size and orientation distribution are enhanced (e.g., increases and decreases, respectively) when film thickness is decreased, ultimately leading to a single-crystal-like behavior for 220 nm thick PEO films of mass 8000 g/mol. Interestingly, this fine microstructure is partially retained after melting and subsequent-cooling back to ambient temperature for the highest molecular weight polymer allowing, in this particular case, to significantly decrease the distribution of crystal orientation obtained after crystallization using the thermal gradient technique.
Why iron oxide nanoflowers are great candidates for magnetic hyperthermia

General information
State: Published
Organizations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Universidad de Cantabria, Technische Universität Braunschweig, Physikalisch-Technische Bundesanstalt, Uppsala University, University College London, AGH University of Science and Technology, Chalmers University of Technology, Micromod Partikeltechnologie GmbH, Institut Laue-Langevin, RISE Acreo
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Main Research Area: Technical/natural sciences

X-ray diffraction microscopy based on refractive optics
A formalism is presented for dark-field X-ray microscopy using refractive optics. The new technique can produce three-dimensional maps of lattice orientation and axial strain within millimetre-sized sampling volumes and is particularly suited to in situ studies of materials at hard X-ray energies. An objective lens in the diffracted beam magnifies the image and acts as a very efficient filter in reciprocal space, enabling the imaging of individual domains of interest with a resolution of 100 nm. Analytical expressions for optical parameters such as numerical aperture, vignetting, and the resolution in both direct and reciprocal spaces are provided. It is shown that the resolution function in reciprocal space can be highly anisotropic and varies as a function of position in the field of view. Inserting a square aperture in front of the objective lens facilitates disjunct and space-filling sampling, which is key for three-dimensional reconstruction and analysis procedures based on the conservation of integrated intensity. A procedure for strain scanning is presented. Finally the formalism is validated experimentally at an X-ray energy of 17 keV.

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Zero-order filter for diffractive focusing of de Broglie matter waves
The manipulation of neutral atoms and molecules via their de Broglie wave properties, also referred to as de Broglie matter wave optics, is relevant for several fields ranging from fundamental quantum mechanics tests and quantum metrology to measurements of interaction potentials and new imaging techniques. However, there are several challenges. For example, for diffractive focusing elements, the zero-order beam provides a challenge because it decreases the signal contrast. Here we present the experimental realization of a zero-order filter, also referred to as an order-sorting aperture for de Broglie matter wave diffractive focusing elements. The zero-order filter makes it possible to measure even at low beam intensities. We present measurements of zero-order filtered, focused, neutral helium beams generated at source stagnation pressures between 11 and 81 bars. We show that for certain conditions the atom focusing at lower source stagnation pressures (broader velocity distributions) is better than what has previously been predicted. We present simulations with the software ray-tracing simulation package MCSTAS using a realistic helium source configuration, which gives very good agreement with our measurements.
Advanced microstructural analysis of cyclically deforming metallic materials towards lifetime improvement

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, Deutsches Elektronen-Synchrotron
Authors: Diederichs, A. M. (Intern), Lienert, U. (Ekstern), Poulsen, H. F. (Intern), Pantleon, W. (Intern)
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Sustain Abstract M-1
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Advanced Neutron Moderators for the ESS

Thermal and cold neutrons are used in a wide array of different experiments investigating the sub-micrometer properties of matter. Neutrons are typically produced at reactor or spallation sources and subsequently cooled to the wanted thermal or cold energy levels by employing neutron moderators. The main increases in thermal and cold intensity are achieved by upscaling the power density of reactors or proton beam power of spallation sources. Reactor development saturated in the 1960s with the construction of the continuous, compact, high-power-density reactors HFIR, Oak Ridge, and ILL, Grenoble. Today these sources are still the most intense neutron sources. The short-pulsed sources SNS and J-PARC are the most powerful spallation sources in the world; although less intense than ILL and HFIR, these sources provide more useful neutrons because of their pulsed beam structure.

This thesis focuses on the European Spallation Source (ESS), which is currently being constructed in Lund, Sweden. The ESS will be a long-pulsed spallation source (pulse length 2.86 ms) driven by a 5-MW proton beam impinging on a rotating tungsten target. The ESS will be the world's most intense neutron source in terms of brightness, but it will also be the first spallation source to outperform reactors in terms of the integrated intensity of thermal and cold neutrons. Experiments at modern facilities use less than one millionth of the neutrons created in neutron source. Much of this inefficiency can be attributed to the moderator system. The imperfections of moderator systems originate from the highly isotropic slowing-down and thermalizing processes, premature leakage (fast neutron escape), neutron absorption and suboptimal geometrical congruations. The inefficiency of moderator systems implies a potential gain in efficiency for neutron sources, which generates an interest in moderator development. Many facilities have proposed and applied advanced moderator concepts to better utilize the produced neutrons. The topic of this thesis is the study of these advanced moderator concepts.

Chapters 1 to 6 briefly summarize the historical development of neutron sources. The ESS is briefly introduced. Then the governing physics is outlined as well as the main principles behind neutron sources and advanced moderators. Chapters 7 to 10 (further detailed below) present novel work in the form of three papers (two published articles, one submitted) and two conference proceedings.

Chapter 7 comprises two conference proceedings and describes the development from the moderator system at the ESS suggested in the Technical Design Report (TDR) to the new moderator baseline (accepted in March 2015), known as the butterfly moderator. The chapter outlines the development process from TDR through the pancake moderator and to the butterfly moderator, and presents various key results. Ultimately, it is shown how this redesign and optimization results in a significant increase in cold and thermal brightness relative to the TDR proposal. Chapter 8 is a study in which MCNPX simulations are transferred to ROOT and analyzed. A method for reconstructing the full emission distribution of the moderator brightness is developed. The ESS pancake moderator (and butterfly moderator in the sub-appendix) is studied. The brightness distributions are fitted to analytical functions that have been implemented in McStas. This enables more precise predictions of the expectations from ESS, which is not only a key requirement for experiments at ESS but also enables neutron instruments to be significantly better optimized before their construction. This, in turn, is expected to contribute significantly to the overall quality of the ESS.

Chapter 9 suggests a novel type of broad-spectrum moderator. This moderator concept is based on the idea that heavy metals, such as lead and bismuth, are inefficient moderator materials. The article investigates this idea through enriched 208Pb. The article shows that the inability of these materials to moderate can be exploited to design a moderator that reflects neutrons from surrounding moderators of different spectral temperatures, with little change in energy. This results in the emission of a broad neutron spectrum (or multiple spectra) from the lead element. Since lead can also serve as a reflector filter, the geometry can be configured such that the broadspectrum lead moderator acts as a reflector filter for a cold moderator positioned behind it, thus increasing the neutron yield below the lead Bragg edge whilst still producing a broad spectrum of neutrons.

Chapter 10 is an experimental paper carried out in the framework of the LENS collaboration. The experiment investigates the concept of a single-crystal reflector filter - a reflector filter that also transmit neutrons in the thermal energy range because of the delta-function-like Bragg edge in a single crystal. The experiment compares single-crystal sapphire, sapphire powder and void. Sapphire was used, since no other single-crystal candidates (diamond, pyrolytic graphite and lithium fluoride) could be obtained within the cost and time constraints of the experiment. Unfortunately, sapphire does not notably increase neutron yield, but the experiment proves the viability of a single-crystal reflector filter and indicates a potential regain of the thermal neutrons lost to a conventional reflector filter, with little or no loss of the cold neutrons below the Bragg edge.

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Organisations: Radiation Physics, Center for Nuclear Technologies, Department of Physics, Neutrons and X-rays for Materials Physics
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Original language: English
Main Research Area: Technical/natural sciences
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A model for non-thermalized neutron spectra emitted from para-hydrogen

At spallation and reactor cold neutron sources, neutrons are cooled by moderators. At high power neutron sources, such as the Japan Proton Accelerator Research Complex (JPARC), European Spallation Source (ESS) and the Spallation Neutron Source (SNS) only few moderator materials are practical, due to the high radiation environment near the moderator and cooling demands. One of the very popular materials, used at J-PARC and planned for ESS, is the spin singlet state of H2, para-hydrogen. This study assesses the non-Maxwellian neutron spectral structure achieved in para-hydrogen moderators, which is due to the complexity of the inelastic scattering cross section below 50 meV. The analytical description of a thermalized spectrum with slowing down components are discussed, then a formula is developed which is a good description of this non-equilibrium para-hydrogen neutron spectrum. These analytical descriptions are fitted to the thermal and cold neutron spectra expected at the European Spallation Source according to the baseline configuration, as described in the Technical Design Report (TDR). The results of the fits have been implemented in McStas 2.0 and is used throughout the ESS instrumentation community. Though not shown here it is worth noting that the spectra for different heights of moderators in the more recent ESS geometry have also been fitted to this para-hydrogen spectrum model, the fits have been implemented and released in McStas 2.1.

A multiple length scale description of the mechanism of elastomer stretching

Conventionally, the stretching of rubber is modeled exclusively by rotations of segments of the embedded polymer chains; i.e. changes in entropy. However, models have not been tested on all relevant length scales due to a lack of appropriate probes. Here we present a universal X-ray based method for providing data on the structure of rubbers in the 2-50 angstrom range. First results relate to the elongation of a silicone rubber. We identify several non-entropic contributions to the free energy and describe the associated structural changes. By far the largest contribution comes from structural changes within the individual monomers, but among the contributions is also an elastic strain, acting between chains, which is 3-4 orders of magnitude smaller than the macroscopic strain, and of the opposite sign, i.e. extension of polymer chains in the direction perpendicular to the stretch. This may be due to trapped entanglements relaxing to positions close to the covalent crosslinks.
An analytic mapping property of the Dirichlet-to-Neumann operator in Helmholtz boundary problems

The analytic version of microlocal analysis shows that if the boundary and the Dirichlet datum of a Helmholtz boundary value problem are real-analytic, then so is the corresponding Neumann datum. However, the domain of analytic continuation of the Neumann datum is, in general, unknown. We shall here relate, in terms of explicit estimates, the domains of analytic continuation of Dirichlet and Neumann boundary data for Helmholtz problems in two or more independent variables, and in neighbourhoods of planar pieces of the boundary. For this purpose, we shall characterise a special subspace of the standard pseudodifferential operators with real-analytic symbols, to which the Dirichlet-to-Neumann operator belongs. The result can be applied in the estimation of the domain of analytic continuation of solutions across planar pieces of the boundary.
A Spectral Geometrical Model for Compton Scatter Tomography Based on the SSS Approximation

The forward model of single scatter in the Positron Emission Tomography for a detector system possessing an excellent spectral resolution under idealized geometrical assumptions is investigated. This model has the form of integral equations describing a flux of photons emanating from the same annihilation event and undergoing a single scattering at a certain angle. The equations for single scatter calculation are derived using the Single Scatter Simulation approximation. We show that the three-dimensional slice-by-slice filtered backprojection algorithm is applicable for scatter data inversion provided some assumptions on the attenuation map are justified.

Atomistic characterization of the active-site solvation dynamics of a model photocatalyst

The interactions between the reactive excited state of molecular photocatalysts and surrounding solvent dictate reaction mechanisms and pathways, but are not readily accessible to conventional optical spectroscopic techniques. Here we report an investigation of the structural and solvation dynamics following excitation of a model photocatalytic molecular system \(\text{Ir}_2(\text{dimen})_4^{2+}\), where dimen is para-diisocyanomenthane. The time-dependent structural changes in this model photocatalyst, as well as the changes in the solvation shell structure, have been measured with ultrafast diffuse X-ray scattering and simulated with Born-Oppenheimer Molecular Dynamics. Both methods provide direct access to the solute-solvent pair distribution function, enabling the solvation dynamics around the catalytically active iridium sites to be robustly characterized. Our results provide evidence for the coordination of the iridium atoms by the acetonitrile solvent and demonstrate the viability of using diffuse X-ray scattering at free-electron laser sources for studying the dynamics of photocatalysis.
A two-stage model of rough-interface scattering for embedded nano-structures

We decompose scattering by nanostructures on rough substrates into two surface transfer functions: one heuristic, computed for the bare substrate from experimental BRDF data, and the other sparse and constructed for nanostructures on smooth surfaces. We explore numerically the performance and the commutativity of this approach.
Blue emitting organic semiconductors under high pressure: status and outlook

This review describes essential optical and emerging structural experiments that use high GPa range hydrostatic pressure to probe physical phenomena in blue-emitting organic semiconductors including π-conjugated polyfluorene and related compounds. The work emphasizes molecular structure and intermolecular self-organization that typically determine transport and optical emission in π-conjugated oligomers and polymers. In this context, hydrostatic pressure through diamond anvil cells has proven to be an elegant tool to control structure and interactions without chemical intervention. This has been highlighted by high pressure optical spectroscopy whilst analogous x-ray diffraction experiments remain less frequent. By focusing on a class of blue-emitting π-conjugated polymers, polyfluorenes, this article reviews optical spectroscopic studies under hydrostatic pressure, addressing the impact of molecular and intermolecular interactions on optical excitations, electron-phonon interaction, and changes in backbone conformations. This picture is connected to the optical high pressure studies of other π-conjugated systems and emerging x-ray scattering experiments from polyfluorenes which provides a structure-property map of pressure-driven intra- and interchain interactions. Key obstacles to obtain further advances are identified and experimental methods to resolve them are suggested.
Butterfly Deformation Modes in a Photoexcited Pyrazolate-Bridged Pt Complex Measured by Time-Resolved X-Ray Scattering in Solution

Pyrazolate-bridged dinuclear Pt(II) complexes represent a series of molecules with tunable absorption and emission properties that can be directly modulated by structural factors, such as the Pt-Pt distance. However, direct experimental information regarding the structure of the emissive triplet excited state has remained scarce. Using time-resolved wide-angle X-ray scattering (WAXS), the excited triplet state molecular structure of [Pt(ppy)(μ-t-Bu₂pz)]₂ (ppy = 2-phenylpyridine; t-Bu₂pz = 3,5-di-tert-butylpyrazolate), complex 1, was obtained in a dilute (0.5 mM) toluene solution utilizing the monochromatic X-ray pulses at Beamline 11IDD of the Advanced Photon Source. The excited-state structural analysis of 1 was performed based on the results from both transient WAXS measurements and density functional theory calculations to shed light on the primary structural changes in its triplet metal-metal-to-ligand charge-transfer (MMLCT) state, in particular, the Pt-Pt distance and ligand rotation. We found a pronounced Pt-Pt distance contraction accompanied by rotational motions of ppy ligands toward one another in the MMLCT state of 1. Our results suggest that the contraction is larger than what has previously been reported, but they are in good agreement with recent theoretical efforts and suggest the ppy moieties as targets for rational synthesis aimed at tuning the excited-state structure and properties.

General information
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Web of Science (2017): Indexed yes
Composition-dependent variation of magnetic properties and interstitial ordering in homogeneous expanded austenite

The crystal structure and magnetic properties of austenitic stainless steel with a colossal interstitial content, so-called expanded austenite, are currently not completely understood. In the present work, the magnetic properties of homogeneous samples of expanded austenite, as prepared by lowerature nitriding of thin foils, were investigated with magnetometry and Mössbauer spectroscopy. At room temperature, expanded austenite is paramagnetic for relatively low and for relatively high nitrogen contents ($y_N = 0.13$ and $0.55$, respectively, where $y_N$ is the interstitial nitrogen occupancy), while ferromagnetism is observed for intermediate nitrogen loads. Spontaneous volume magnetostriction was observed in the ferromagnetic state and the Curie temperature was found to depend strongly on the nitrogen content. For the first time, X-ray diffraction evidence for the occurrence of long-range interstitial order of nitrogen atoms in expanded austenite was observed for high nitrogen contents.

General information

State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemistry, X-ray Crystallography, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Micro- and Nanotechnology, Magnetic Systems
DanMAX - The Danish beamline for in situ materials studies at MAX IV

**General information**
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Aarhus University
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DanMAX, synchrotron powder X-ray diffraction, Instrumentation, MAX IV, Materials science, Tomography

**Direct observation of grain rotations during coarsening of a semisolid Al-Cu alloy**
Sintering is a key technology for processing ceramic and metallic powders into solid objects of complex geometry, particularly in the burgeoning field of energy storage materials. The modeling of sintering processes, however, has not kept pace with applications. Conventional models, which assume ideal arrangements of constituent powders while ignoring their underlying crystallinity, achieve at best a qualitative description of the rearrangement, densification, and coarsening of powder compacts during thermal processing. Treating a semisolid Al-Cu alloy as a model system for late-stage sintering—during which densification plays a subordinate role to coarsening—we have used 3D X-ray diffraction microscopy to track the changes in sample microstructure induced by annealing. The results establish the occurrence of significant particle rotations, driven in part by the dependence of boundary energy on crystallographic misorientation. Evidently, a comprehensive model for sintering must incorporate crystallographic parameters into the thermodynamic driving forces governing microstructural evolution.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Ulm, University of Copenhagen, Japan Synchrotron Radiation Research Institute
Authors: Dake, J. M. (Ekstern), Oddershede, J. (Intern), Sørensen, H. O. (Ekstern), Werz, T. (Ekstern), Shatto, J. C. (Ekstern), Uesugi, K. (Ekstern), Schmidt, S. (Intern), Krill III, C. E. (Ekstern)
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Direct observation of the thermal demagnetization of magnetic vortex structures in nonideal magnetite recorders: Thermal Demagnetization of Vortex States

The thermal demagnetization of pseudo-single-domain (PSD) magnetite (Fe$_3$O$_4$) particles, which govern the magnetic signal in many igneous rocks, is examined using off-axis electron holography. Visualization of a vortex structure held by an individual Fe$_3$O$_4$ particle (~250nm in diameter) during in situ heating is achieved through the construction and examination of magnetic-induction maps. Stepwise demagnetization of the remanence-induced Fe$_3$O$_4$ particle upon heating to above the Curie temperature, performed in a similar fashion to bulk thermal demagnetization measurements, revealed that its vortex state remains stable under heating close to its unblocking temperature and is recovered upon cooling with the same or reversed vorticity. Hence, the PSD Fe3O4 particle exhibits thermomagnetic behavior comparable to a single-domain carrier, and thus, vortex states are considered reliable magnetic recorders for paleomagnetic investigations.
Dual strain mechanisms in a lead-free morphotropic phase boundary ferroelectric

Electromechanical properties such as $d_{33}$ and strain are significantly enhanced at morphotropic phase boundaries (MPBs) between two or more different crystal structures. Many actuators, sensors and MEMS devices are therefore systems with MPBs, usually between polar phases in lead (Pb)-based ferroelectric ceramics. In the search for Pb-free alternatives, systems with MPBs between polar and non-polar phases have recently been theorized as having great promise. While such an MPB was identified in rare-earth (RE) modified bismuth ferrite (BFO) thin films, synthesis challenges have prevented its realization in ceramics. Overcoming these, we demonstrate a comparable electromechanical response to Pb-based materials at the polar-to-non-polar MPB in Sm modified BFO. This arises from ‘dual’ strain mechanisms: ferroelectric/ferroelastic switching and a previously unreported electric-field induced transition of an anti-polar intermediate phase. We show that intermediate phases play an important role in the macroscopic strain response, and may have potential to enhance electromechanical properties at polar-to-non-polar MPBs.
Effect of side-chain asymmetry on the intermolecular structure and order-disorder transition in alkyl-substituted polyfluorenes

We study relations among the side-chain asymmetry, structure, and order-disorder transition (ODT) in hairy-rod-type poly(9,9-dihexylfluorene) (PF6) with two identical side chains and atactic poly(9-octyl-9-methyl-fluorene) (PF1-8) with two different side chains per repeat. PF6 and PF1-8 organize into alternating side-chain and backbone layers that transform into an isotropic phase at TODT(PF6) and TODT(PF1−8). We interpret polymers in terms of monodisperse and bidisperse brushes and predict scenarios TODT<TODTbi and TODT∼TODTbi for high and low grafting densities (the side-chain length above or below the average grafting distance). Calorimetry and x-ray scattering indicate the condition TODT(PF6)∼TODTbi(PF1−8) following the low grafting prediction. PF6 side chains coming from the alternating backbone layers appear as two separate layers with thickness H(PF6), whereas PF1-8 side chains appear as an indistinguishable bilayer with a half thickness Hbilayer(PF1−8)/2=H(PF6). The low grafting density region is structurally possible but not certain for PF6 and confirmed for PF1-8.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, DSM Research, University of Helsinki, Lund University, Bergische Universität Wuppertal
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Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
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Electron Transfer and Solvent-Mediated Electronic Localization in Molecular Photocatalysis

This work provides a detailed mechanism for electron transfer in a heterodinuclear complex designed as a model system in which to study homogeneous molecular photocatalysis. With efficient Born–Oppenheimer molecular dynamics simulations, we show how intermediate, charge-separated states can mediate the electron transfer. We observe how Jahn–Teller distortion effects play out in solution, when the molecule has energetically close-lying states, and how this distortion is averaged out in the thermal sampling. Finally, we demonstrate how the solvent helps stabilize and localize the separated charge. The information on the electronic configuration and separate states is of key importance for designing next-generation photocatalysts.
Experimental characterization of a prototype secondary spectrometer for vertically scattering multiple energy analysis at cold-neutron triple axis spectrometers

A thorough experimental characterization of a multiplexing backend with multiple energy analysis on a cold-neutron triple axis spectrometer (cTAS) is presented. The prototype employs two angular segments (2 theta-segments) each containing five vertically scattering analyzers (energy channels), which simultaneously probe an energy transfer range of 2 meV at the corresponding two scattering angles. The feasibility and strength of such a vertically scattering multiple energy analysis setup is clearly demonstrated. It is shown, that the energy resolution near the elastic line is comparable to the energy resolution of a standard cTAS. The dispersion relation of the antiferromagnetic excitations in MnF2 has been mapped out by performing constant energy transfer maps. These results show that the tested setup is virtually spurious free. In addition, focusing effects due to (mis)matching of the instrumental resolution ellipsoid to the excitation branch are clearly evident. (C) 2016 Elsevier B.V. All rights reserved.
Femtosecond X-ray absorption and emission spectroscopy on ZnO nanoparticles in solution

We have performed femtosecond X-ray spectroscopy measurements after UV photoexcitation of a colloidal solution of ZnO nanoparticles. The results indicate sub-ps hole trapping at oxygen vacancies with shallowly-trapped electrons in the conduction band.

General information

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Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated \([\text{Co(terpy)}_2]^{2+}\)

We study the structural dynamics of photoexcited \([\text{Co(terpy)}_2]^{2+}\) in an aqueous solution with ultrafast x-ray diffuse scattering experiments conducted at the Linac Coherent Light Source. Through direct comparisons with density functional theory calculations, our analysis shows that the photoexcitation event leads to elongation of the Co-N bonds, followed by coherent Co-N bond length oscillations arising from the impulsive excitation of a vibrational mode dominated by the symmetrical stretch of all six Co-N bonds. This mode has a period of 0.33 ps and decays on a subpicosecond time scale. We find that the equilibrium bond-elongated structure of the high spin state is established on a single-picosecond time scale and that this state has a lifetime of ∼7 ps.

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Scopus rating (2013): SJR 5.674 SNIP 2.796 CiteScore 7.46
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
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Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 6.252 SNIP 2.886 CiteScore 7.02
FeNi/\gamma-Al_2O_3 Egg-shell Catalyst for H_2 Generation by Ammonia Decomposition

**FeNi/\gamma-Al_2O_3 Egg-shell Catalyst for H_2 Generation by Ammonia Decomposition**

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Neutrons and X-rays for Materials Physics
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Electronic versions: C.Damsgaard_NSC2016_poster.pdf

**Bibliographical note**
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Source-ID: 127045887
Publication: Research - peer-review > Poster – Annual report year: 2016
Full-field hard x-ray microscopy with interdigitated silicon lenses

Full-field x-ray microscopy using x-ray objectives has become a mainstay of the biological and materials sciences. However, the inefficiency of existing objectives at x-ray energies above 15 keV has limited the technique to weakly absorbing or two-dimensional (2D) samples. Here, we show that significant gains in numerical aperture and spatial resolution may be possible at hard x-ray energies by using silicon-based optics comprising ‘interdigitated’ refractive silicon lenslets that alternate their focus between the horizontal and vertical directions. By capitalizing on the nano-manufacturing processes available to silicon, we show that it is possible to overcome the inherent inefficiencies of silicon-based optics and interdigitated geometries. As a proof-of-concept of Si-based interdigitated objectives, we demonstrate a prototype interdigitated lens with a resolution of ≈255 nm at 17 keV.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, DTU Danchip, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
Pages: 460-464
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Main Research Area: Technical/natural sciences

Publication information
Journal: Optics Communications
Volume: 359
ISSN (Print): 0030-4018
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.65 SJR 0.633 SNIP 0.924
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.711 SNIP 0.987 CiteScore 1.62
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.719 SNIP 1.058 CiteScore 1.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.746 SNIP 1.175 CiteScore 1.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.813 SNIP 1.151 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.814 SNIP 1.21 CiteScore 1.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.935 SNIP 1.18
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.047 SNIP 1.218
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.139 SNIP 1.24
Heterogeneous grain-scale response in ferroic polycrystals under electric field

Understanding coupling of ferroic properties over grain boundaries and within clusters of grains in polycrystalline materials is hindered due to a lack of direct experimental methods to probe the behaviour of individual grains in the bulk of a material. Here, a variant of three-dimensional X-ray diffraction (3D-XRD) is used to resolve the non-180° ferroelectric domain switching strain components of 191 grains from the bulk of a polycrystalline electro-ceramic that has undergone an electric-field-induced phase transformation. It is found that while the orientation of a given grain relative to the field direction has a significant influence on the phase and resultant domain texture, there are large deviations from the average behaviour at the grain scale. It is suggested that these deviations arise from local strain and electric field neighbourhoods being highly heterogeneous within the bulk polycrystal. Additionally, the minimisation of electrostatic potentials at the grain boundaries due to interacting ferroelectric domains must also be considered. It is found that the local grain-scale deviations average out over approximately 10–20 grains. These results provide unique insight into the grain-scale interactions of ferroic materials and will be of value for future efforts to comprehensively model these and related materials at that length-scale.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility, Ulsan National Institute of Science and Technology
Authors: Daniels, J. E. (Ekstern), Majkut, M. (Intern), Cao, Q. (Ekstern), Schmidt, S. (Intern), Wright, J. (Ekstern), Jo, W. (Ekstern), Oddershede, J. (Intern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 22820
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Imaging ultrafast excited state pathways in transition metal complexes by X-ray transient absorption and scattering using X-ray free electron laser source

This report will describe our recent studies of transition metal complex structural dynamics on the fs and ps time scales using an X-ray free electron laser source, Linac Coherent Light Source (LCLS). Ultrafast XANES spectra at the Ni K-edge of nickel(ii) tetramesitylporphyrin (NiTMP) were measured for optically excited states at a timescale from 100 fs to 50 ps, providing insight into its sub-ps electronic and structural relaxation processes. Importantly, a transient reduced state Ni(i) (π, 3d_x^2-y^2) electronic state is captured through the interpretation of a short-lived excited state absorption on the low-energy shoulder of the edge, which is aided by the computation of X-ray transitions for postulated excited electronic states. The observed and computed inner shell to valence orbital transition energies demonstrate and quantify the influence of the electronic configuration on specific metal orbital energies. A strong influence of the valence orbital occupation on the inner shell orbital energies indicates that one should not use the transition energy from 1s to other orbitals to draw conclusions about the d-orbital energies. For photocatalysis, a transient electronic configuration could influence d-orbital energies up to a few eV and any attempt to steer the reaction pathway should account for this to ensure that external energies can be used optimally in driving desirable processes. NiTMP structural evolution and the influence of the porphyrin macrocycle conformation on relaxation kinetics can be likewise inferred from this study.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory, Northwestern University, University of Washington, Argonne National Laboratory
Authors: Chen, L. X. (Ekstern), Shelby, M. L. (Ekstern), Lestrange, P. J. (Ekstern), Jackson, N. E. (Ekstern), Haldrup, K. (Intern), Mara, M. W. (Ekstern), Stickrath, A. B. (Ekstern), Zhu, D. (Ekstern), Lemke, H. (Ekstern), Chollet, M. (Ekstern), Hoffman, B. M. (Ekstern), Li, X. (Ekstern)
Number of pages: 20
Incorporation of a Cationic Conjugated Polyelectrolyte CPE within an Aqueous Poly(vinyl alcohol) Sol
We report on a multiscale polymer-within-polymer structure of the cationic conjugated polyelectrolyte poly[9,9-bis(6-N,N,N-trimethylammonium)hexyl]fluorene phenylene] (HTMAPFP) in aqueous poly(vinyl alcohol). (PVA) sol. Molecular dynamics simulations and small-angle neutron scattering (SANS) data show that HTMA-PFP forms aggregates in water but becomes entangled by PVA (with a 1:1 molar ratio of HTMA-PFP to PVA) and eventually immersed in PVA clusters (with the ratio 1:4). This is attributed to the hydrophobic hydrophilic balance. Contrast variation data with regular and deuterated PVA support a rigid body model, where HTMA-PFP is confined as locally isolated, but closely located, chains within PVA clusters, which alter correlation distances within the system. These results are supported by enhanced photoluminescence (PL) and ionic conductivity which, together with a red-shift in UV/vis absorption spectra, indicate the breakup of HTMA-PFP aggregates upon PVA addition.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Coimbra, Universidad Miquel Hernandez de Elche
Number of pages: 13
Pages: 9119-9131
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecules
Volume: 49
Issue number: 23
ISSN (Print): 0024-9297
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.76 SJR 2.557 SNIP 1.507
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.407 SNIP 1.638 CiteScore 5.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.534 SNIP 1.721 CiteScore 5.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.576 SNIP 1.754 CiteScore 6.09
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.779 SNIP 1.58 CiteScore 5.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.556 SNIP 1.593 CiteScore 5.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.51 SNIP 1.51
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Induction-Heated Hydrogen Production

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Neutrons and X-rays for Materials Physics, Haldor Topsoe AS
Authors: Wismann, S. T. (Intern), Chorkendorff, I. (Intern), Frandsen, C. (Intern), M. Mortensen, P. (Ekstern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
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Layered Surface Detection in Micro-CT Tetra Pak Data

General information
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Organisations: Department of Applied Mathematics and Computer Science, Statistics and Data Analysis, Department of Physics, Neutrons and X-rays for Materials Physics, Image Analysis & Computer Graphics, Tetra Pak Packaging Solutions AB
Number of pages: 3
Publication date: 2016
Magnetic field controlled charge density wave coupling in underdoped YBa$_2$Cu$_3$O$_{6+x}$

The application of magnetic fields to layered cuprates suppresses their high-temperature superconducting behaviour and reveals competing ground states. In widely studied underdoped YBa$_2$Cu$_3$O$_{6+x}$ (YBCO), the microscopic nature of field-induced electronic and structural changes at low temperatures remains unclear. Here we report an X-ray study of the high-field charge density wave (CDW) in YBCO. For hole dopings $\sim 0.123$, we find that a field ($B\sim10$ T) induces additional CDW correlations along the CuO chain (b-direction) only, leading to a three-dimensional (3D) ordered state along this direction at $B\sim15$ T. The CDW signal along the a-direction is also enhanced by field, but does not develop an additional pattern of correlations. Magnetic field modifies the coupling between the CuO$_2$ bilayers in the YBCO structure, and causes the sudden appearance of the 3D CDW order. The mirror symmetry of individual bilayers is broken by the CDW at low and high fields, allowing Fermi surface reconstruction, as recently suggested.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Universität Zürich, University of Birmingham, European Spallation Source ESS AB, Brookhaven National Laboratory, University of British Columbia, University of Bristol, Deutsches Elektronen-Synchrotron
Authors: Chang, J. (Ekstern), Blackburn, E. (Ekstern), Ivashko, O. (Ekstern), Holmes, A. T. (Ekstern), Christensen, N. B. (Intern), Huecker, M. (Ekstern), Liang, R. (Ekstern), Bonn, D. A. (Ekstern), Hardy, W. N. (Ekstern), Rütt, U. (Ekstern), Zimmermann, M. V. (Ekstern), Forgan, E. M. (Ekstern), Hayden, S. M. (Ekstern)
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Article number: 11494
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BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.399 SNIP 2.995
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.364 SNIP 3.053 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.331 SNIP 3.091 CiteScore 10.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.967 SNIP 2.776 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.586 SNIP 2.724 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.122 SNIP 1.544 CiteScore 4.44
ISI indexed (2011): ISI indexed no
Web of Science (2010): Indexed yes
Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction

This thesis presents an in-situ three-dimensional study of the grain-scale response of a prototypical piezoelectric ceramic, barium titanate (BT), to an externally applied electric field. Piezoceramics take advantage of the coupling of electrical and mechanical energies for use in sensors and actuators, found in both common applications such as fuel injectors and specialized applications such as medical imaging equipment. Since piezoceramics are typically used in the polycrystalline state it is important to consider not just the crystal structure but also the role of intergranular effects in the structure-properties relationships. Such effects are difficult to observe using destructive two-dimensional microscopy techniques and averaged over the entire sample in conventional powder diffraction studies. We instead use a combination of nondestructive three-dimensional X-ray diffraction techniques to study the material at the grain scale.

First, we use the intensity ratios of split diffraction peaks to extract grain-scale domain volume fractions for 139 grains. We find that even in the as-processed state there exist unequal volume fractions of each domain type, which we attribute to a heterogeneous local environment at the cubic to tetragonal transition during processing. When a field is applied, we observe a first-order orientation dependence with second order deviations, again attributed to the grain neighbourhood effect. Corellation of this with microstructural parameters such as grain size, neighbour misorientation and position within the sample did not reveal any obvious causes.

Next we develop a novel indexing and refinement method whereby the peak positions of domains are forward projected from crystallographic twinning orientations and the deviation between projected and measured diffraction patterns is minimized to refine domain-scale orientations and lattice parameters. We present the results of refinement for a bulk grain in which the domains are found to be misoriented from perfect crystallographic twins by 0.1-0.3°, suggesting a strained microstructure. The data set was collected by illuminating the entire width of the sample with a box beam, thus it contains a statistically significant number of grains for which domain-scale parameters will be refined in the future.

Maximising electro-mechanical response by minimising grain-scale strain heterogeneity in phase-change actuator ceramics

Phase-change actuator ceramics directly couple electrical and mechanical energies through an electric-field-induced phase transformation. These materials are promising for the replacement of the most common electro-mechanical ceramic, lead zirconate titanate, which has environmental concerns. Here, we show that by compositional modification, we reduce the grain-scale heterogeneity of the electro-mechanical response by 40%. In the materials investigated, this leads to an increase in the achievable electric-field-induced strain of the bulk ceramic of 45%. Compositions of (100-x)Bi0.5Na0.5TiO3-(x)BaTiO3, which initially possess a pseudo-cubic symmetry, can be tuned to undergo phase transformations to combined lower symmetry phases, thus decreasing the anisotropy of the transformation strain. Further, modelling of transformation strains of individual grains shows that minimum grain-scale strain heterogeneity can be achieved by precise control of the lattice distortions and orientation distributions of the induced phases. The current results can be used to guide the design of next generation high-strain electro-mechanical ceramic actuator materials.
Multigrain indexing of unknown multiphase materials

A multigrain indexing algorithm for use with samples comprising an arbitrary number of known or unknown phases is presented. No a priori crystallographic knowledge is required. The algorithm applies to data acquired with a monochromatic beam and a conventional two-dimensional detector for diffraction. Initially, candidate grains are found by searching for crystallographic planes, using a Dirac comb convoluted with a box function as a filter. Next, candidate grains are validated and the unit cell is optimized. The algorithm is validated by simulations. Simulations of 500 cementite grains and similar to 100 reflections per grain resulted in 99.2% of all grains being indexed correctly and 99.5% of the reflections becoming associated with the right grain. Simulations with 200 grains associated with four mineral phases and 50-700 reflections per grain resulted in 99.9% of all grains being indexed correctly and 99.9% of the reflections becoming associated with the right grain. The main limitation is in terms of overlap of diffraction spots and computing time. Potential areas of use include three-dimensional grain mapping, structural solution and refinement studies of complex samples, and studies of dilute phases.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Wejdemann, C. (Intern), Poulsen, H. F. (Intern)
Number of pages: 6
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Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 49
Issue number: 2
ISSN (Print): 0021-8898
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
Multiscale 3D characterization with dark-field x-ray microscopy

Dark-field x-ray microscopy is a new way to three-dimensionally map lattice strain and orientation in crystalline matter. It is analogous to dark-field electron microscopy in that an objective lens magnifies diffracting features of the sample; however,
the use of high-energy synchrotron x-rays means that these features can be large, deeply embedded, and fully mapped in seconds to minutes. Simple reconfiguration of the x-ray objective lens allows intuitive zooming between different scales down to a spatial and angular resolution of 100 nm and 0.001 degrees, respectively. Three applications of the technique are presented—mapping the evolution of subgrains during the processing of plastically deformed aluminum, mapping domains and strain fields in ferroelectric crystals, and the three-dimensional mapping of strain fields around individual dislocations. This ability to directly characterize complex, multiscale phenomena in situ is a key step toward formulating and validating multiscale models that account for the entire heterogeneity of materials.
Noise robustness of a combined phase retrieval and reconstruction method for phase-contrast tomography

Classical reconstruction methods for phase-contrast tomography consist of two stages: phase retrieval and tomographic reconstruction. A novel algebraic method combining the two was suggested by Kostenko et al. [Opt. Express 21, 12185 (2013) [CrossRef], and preliminary results demonstrated improved reconstruction compared with a given two-stage method. Using simulated free-space propagation experiments with a single sample-detector distance, we thoroughly compare the novel method with the two-stage method to address limitations of the preliminary results. We demonstrate that the novel method is substantially more robust toward noise; our simulations point to a possible reduction in counting times by an order of magnitude.
Novel micro-reactor flow cell for investigation of model catalysts using in situ grazing-incidence X-ray scattering

The design, fabrication and performance of a novel and highly sensitive micro-reactor device for performing in situ grazing-incidence X-ray scattering experiments of model catalyst systems is presented. The design of the reaction chamber, etched in silicon on insulator (SIO), permits grazing-incidence small-angle X-ray scattering (GISAXS) in transmission through 10 µm-thick entrance and exit windows by using micro-focused beams. An additional thinning of the Pyrex glass reactor lid allows simultaneous acquisition of the grazing-incidence wide-angle X-ray scattering (GIWAXS). In situ experiments at synchrotron facilities are performed utilizing the micro-reactor and a designed transportable gas feed and analysis system. The feasibility of simultaneous in situ GISAXS/GIWAXS experiments in the novel micro-reactor flow cell was confirmed with CO oxidation over mass-selected Ru nanoparticles.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Individual Nanoparticle Functionality, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Experimental Surface and Nanomaterials Physics, Paul Scherrer Institut
Number of pages: 9
Pages: 455-463
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Synchrotron Radiation
Volume: 23
Issue number: 2
ISSN (Print): 0909-0495
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.593 SNIP 1.578
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.161 SNIP 1.396 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.505 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.473 SNIP 1.687 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.558 SNIP 1.273 CiteScore 2.36
Observing Solvation Dynamics with Simultaneous Femtosecond X-ray Emission Spectroscopy and X-ray Scattering

In liquid phase chemistry dynamic solute solvent interactions often govern the path, ultimate outcome, and efficiency of chemical reactions. These steps involve many-body movements on subpicosecond time scales and thus ultrafast structural tools capable of capturing both intramolecular electronic and structural changes, and local solvent structural changes are desired. We have studied the intra- and intermolecular dynamics of a model chromophore, aqueous [Fe(bpy)3]2+, with complementary X-ray tools in a single experiment exploiting intense XFEL radiation as a probe. We monitored the ultrafast structural rearrangement of the solute with X-ray emission spectroscopy, thus establishing time zero for the ensuing X-ray diffuse scattering analysis. The simultaneously recorded X-ray diffuse scattering attens reveal slower subpicosecond dynamics triggered by the intramolecular structural dynamics of the photoexcited solute. By simultaneous combination of both methods only, we can extract new information about the solvation dynamic processes unfolding during the first picosecond (ps). The measured bulk solvent density increase of 0.2% indicates a dramatic change of the solvation shell around each photoexcited solute, confirming previous ab initio molecular dynamics simulations. Structural changes in the aqueous solvent associated with density and temperature changes occur with similar to 1 ps time constants, characteristic for structural dynamics in water. This slower time scale of the solvent response allows us to directly observe the structure of the excited solute molecules well before the solvent contributions become dominant.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, European XFEL, Paul Scherrer Institut, SLAC National Accelerator Laboratory, Hungarian Academy of Sciences, Lund University, European Synchrotron Radiation Facility
Precipitation pathways for ferrihydrite formation in acidic solutions

Iron oxides and oxyhydroxides form via Fe$^{3+}$ hydrolysis and polymerization in many aqueous environments, but the pathway from Fe$^{3+}$ monomers to oligomers and then to solid phase nuclei is unknown. In this work, using combined X-ray, UV-vis, and Mossbauer spectroscopic approaches, we were able to identify and quantify the long-time sought ferric speciation over time during ferric oxyhydroxide formation in partially-neutralized ferric nitrate solutions ([Fe$^{3+}$] = 0.2 M, 1.8 <pH <3). Results demonstrate that Fe exists mainly as Fe(H$_2$O)$_6^{3+}$, mu-oxo aquo dimers and ferrihydrite, and that with time, the mu-oxo dimer decreases while the other two species increase in their concentrations. No larger Fe oligomers were detected. Given that the structure of the mu-oxo dimer is incompatible with those of all Fe oxides and oxyhydroxides, our results suggest that reconfiguration of the mu-oxo dimer structure occurs prior to further condensation leading up to the nucleation of ferrihydrite. The structural reconfiguration is likely the rate-limiting step involved in the nucleation process.
In this paper we present recent achievements in the field of investigation of the local, electronic and magnetic structure of the matter under extreme conditions of pressure and temperature. These results were obtained thanks to the coupling of a compact laser heating system to the energy-dispersive XAS technique available on the ID24 beamline at the ESRF synchrotron. The examples chosen concern the melting and the liquid structure of 3d metals and alloys under high pressures (HPs) and the observation of temperature-induced spin crossover in FeCO$_3$ at HP.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility, Sorbonne Universités, Ehime University
Authors: Torchio, R. (Ekstern), Boccato, S. (Ekstern), Cerantola, V. (Ekstern), Morard, G. (Ekstern), Irifune, T. (Ekstern), Kantor, I. (Intern)
Number of pages: 10
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.437 SNIP 0.724 CiteScore 1.12
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Quantifying the onset of recrystallization in deformed metals using x-rays

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Ahl, S. R. (Intern), Simons, H. (Intern), Poulsen, H. F. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-4
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
Reversible Polarization Rotation in Epitaxial Ferroelectric Bilayers

Polarization rotation engineering is a promising path to giant dielectric and electromechanical responses in ferroelectric materials and devices. This work demonstrates robust and reversible in- to out-of-plane polarization rotation in ultrathin (nanoscale) epitaxial (001) tetragonal PbZr$_{0.3}$Ti$_{0.7}$O$_3$ (PZT-T)/rhombohedral PbZr$_{0.55}$Ti$_{0.45}$O$_3$ (PZT-R) ferroelectric bilayers. An underlying 20 nm thick PZT-R layer reduces the symmetry in a 5 nm thick PZT-T layer by imposing an in-plane tensile strain while simultaneously decoupling the PZT-T layer from the substrate. This prevents clamping and facilitates large-scale polarization rotation switching (~60 μC cm$^{-2}$) and an effective d$_{33}$ response 500% (~250 pm V$^{-1}$) larger than the PZT-R layer alone. Furthermore, this enhancement is stable for more than 10$^7$ electrical switching cycles. These bilayers present a simple and highly controllable means to design and optimize rotational polar systems as an alternate to traditional composition-based approaches. The precise control of the subtle interface-driven interactions between the lattice and the external factors that control polarization opens a new door to enhanced—or completely new—functional properties.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, Pennsylvania State University
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Journal: Advanced Materials Interfaces
Article number: 1600444
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Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.57 SJR 1.451 SNIP 0.819
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.131 SNIP 0.63 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Original language: English
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Source-ID: 2306762657
Publication: Research - peer-review › Journal article – Annual report year: 2016

Robust structural identification via polyhedral template matching

Successful scientific applications of large-scale molecular dynamics often rely on automated methods for identifying the local crystalline structure of condensed phases. Many existing methods for structural identification, such as common neighbour analysis, rely on interatomic distances (or thresholds thereof) to classify atomic structure. As a consequence they are sensitive to strain and thermal displacements, and preprocessing such as quenching or temporal averaging of the atomic positions is necessary to provide reliable identifications. We propose a new method, polyhedral template matching (PTM), which classifies structures according to the topology of the local atomic environment, without any ambiguity in the classification, and with greater reliability than e.g. common neighbour analysis in the presence of thermal fluctuations. We demonstrate that the method can reliably be used to identify structures even in simulations near the melting point, and that it can identify the most common ordered alloy structures as well. In addition, the method makes it easy to identify the local lattice orientation in polycrystalline samples, and to calculate the local strain tensor. An implementation is made available under a Free and Open Source Software license.

General information
State: Published
Self-assembled systems of water soluble metal 8-hydroxyquinolates with surfactants and conjugated polyelectrolytes

We have studied the interaction of 8-hydroxyquinoline-5-sulfonate (8-HQS) with the metal ions Al(III) and Zn(II) in aqueous solution in the presence of tetraalkylammonium surfactants using UV/vis absorption, fluorescence, NMR spectroscopy and electrical conductivity measurements, complemented by DFT calculations and molecular dynamics (MD) simulations. Under appropriate conditions, complexes between 8-HQS and metal ions form rapidly, and have similar electronic, spectroscopic and photophysical properties to the corresponding metal quinolates, such as Alq3. These interact with the cationic surfactants, leading to marked increases in fluorescence intensity. However, significant differences are seen in the behavior of the two metal ions. With aluminium, a stable [Al(8-QS)3]3− anion is formed, and interacts, predominantly through electrostatic interactions, with the surfactant, without disrupting the metal ion coordination sphere. In contrast, with Zn(II), there is a competition between the metal ion and surfactants in the interaction with 8-HQS, although the [Zn(8-QS)2(H2O)2]2− species is stable at appropriate pH and surfactant concentration. The studies are extended to systems with the conjugated polyelectrolyte (CPE) poly-(9,9-bis(6-N, N-trimethylammonium) hexyl)-fluorene-phenylene bromide (HTMA-PFP), which has a similar alkylammonium chain to the surfactants. Mixing metal salt, 8-HQS and HTMA-PFP in the presence of a nonionic surfactant leads to the formation of a metal complex/CPE supramolecular assembly between the conjugated polyelectrolyte and the metal/8-HQS complex, as demonstrated by electronic energy transfer. The potential of these systems in sensing, light harvesting, and electron injection/transport layers in organic semiconductor devices is discussed.

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Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Simulating X-ray telescopes with McXtrace: A case study of ATHENA’s optics

General information
State: Published
Organisations: National Space Institute, Astrophysics and Atmospheric Physics, Department of Physics, Neutrons and X-rays for Materials Physics, National Institute for Astrophysics, University of Copenhagen, European Space Agency
Authors: Della Monica Ferreira, D. (Intern), Bergbäck Knudsen, E. (Intern), Westergaard, N. J. S. (Intern), Christensen, F. E. (Intern), Massahi, S. (Intern), Shortt, B. (Ekstern), Spiga, D. (Ekstern), Solstade, M. (Ekstern), Lefmann, K. (Ekstern)
Number of pages: 8
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Simulation and modeling of silicon pore optics for the ATHENA X-ray telescope

General information
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Organisations: National Space Institute, Astrophysics and Atmospheric Physics, Department of Physics, Neutrons and X-rays for Materials Physics, National Institute for Astrophysics, European Space Agency
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Article number: 990576
Main Research Area: Technical/natural sciences
Conference: Space Telescopes and Instrumentation 2016, Edinburgh, United Kingdom, 26/06/2016 - 26/06/2016
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Bibliographical note
Downloading of the abstract is permitted for personal use only.
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Simultaneous resonant x-ray diffraction measurement of polarization inversion and lattice strain in polycrystalline ferroelectrics

Structure-property relationships in ferroelectrics extend over several length scales from the individual unit cell to the macroscopic device, and with dynamics spanning a broad temporal domain. Characterizing the multi-scale structural origin of electric field-induced polarization reversal and strain in ferroelectrics is an ongoing challenge that so far has obscured its fundamental behaviour. By utilizing small intensity differences between Friedel pairs due to resonant scattering, we demonstrate a time-resolved X-ray diffraction technique for directly and simultaneously measuring both lattice strain and, for the first time, polarization reversal during in-situ electrical perturbation. This technique is demonstrated for BaTiO$_3$-BiZn$_{0.5}$Ti$_{0.5}$O$_3$ (BT-BZT) polycrystalline ferroelectrics, a prototypical lead-free piezoelectric with an ambiguous switching mechanism. This combines the benefits of spectroscopic and diffraction-based measurements into a single and robust technique with time resolution down to the ns scale, opening a new door to in-situ structure-property characterization that probes the full extent of the ferroelectric behaviour.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Siegen, North Carolina State University, Oregon State University, European Synchrotron Radiation Facility
Authors: Gorfman, S. (Ekstern), Simons, H. (Intern), Iamsasri, T. (Ekstern), Prasertpalichat, S. (Ekstern), Cann, D. P. (Ekstern), Choe, H. (Ekstern), Pietsch, U. (Ekstern), Watier, Y. (Ekstern), Jones, J. L. (Ekstern)
Number of pages: 9
Publication date: 2016
Structural dynamics of solvated metal complexes with anisotropy-enhanced X-ray scattering

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Biasin, E. (Intern), Nielsen, M. M. (Intern), Haldrup, K. (Intern)
Number of pages: 182
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Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
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Projects:
Structural dynamics of solvated metal complexes with anisotropy-enhanced X-ray scattering
Publication: Research › Ph.D. thesis – Annual report year: 2016
Temperature dependent piezoelectric response and strain-electric-field hysteresis of rare-earth modified bismuth ferrite ceramics

The rare-earth (RE)-modified bismuth ferrite (BiFeO₃ or BFO) family of ferroelectrics have uncomplicated lead-free chemistries and simple perovskite structures. Due to the high Curie transition temperature of the parent BiFeO₃ perovskite (similar to 830 °C), they are promising piezoelectric materials for use at elevated temperatures. However, the influence of the specific RE species on the electromechanical behavior at high temperatures and above the coercive electric-field is not widely reported. Here, structural analysis over multiple length scales using X-ray diffraction, transmission electron microscopy and piezoresponse force microscopy is coupled with a high electric-field cycling study and in situ converse d₃₃ measurements up to 325 °C for three RE-BFO ceramic compositions, Bi₀.₈₆Sm₀.₁₄FeO₃, Bi₀.₈₈Gd₀.₁₂FeO₃ and Bi₀.₉₁Dy₀.₀₉FeO₃. The ceramics exhibit different phase assemblages with varying amounts of polar rhombohedral R3c and intermediate antipolar orthorhombic Pbam phases as a function of the RE species. During electric-field cycling at electric-fields with amplitudes of 160 kV cm⁻¹, peak-to-peak strains of 0.23-0.27% are reached for all three compositions. However, there are qualitative differences in the field-induced strain and electric current behavior as a function of electric-field cycling and the materials exhibit an electrical-history dependent behavior. Bi₀.₉₁Dy₀.₀₉FeO₃ possesses an improved d₃₃ stability as a function of temperature relative to the parent BFO perovskite and the highest depolarization temperature among the three RE-BFO compositions, with a stable d₃₃ of similar to 22 pC N⁻¹ up to 325 °C.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Josef Stefan Institute, University of Sheffield, University of New South Wales, Politecnico di Torino
Authors: Walker, J. (Ekstern), Ursic, H. (Ekstern), Bencan, A. (Ekstern), Malic, B. (Ekstern), Simons, H. (Intern), Reaney, I. (Ekstern), Viola, G. (Ekstern), Nagarajan, V. (Ekstern), Rojac, T. (Ekstern)
Number of pages: 10
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Scopus rating (2015): SJR 1.751 SNIP 1.577 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.505 SNIP 1.36 CiteScore 4.64
Web of Science (2014): Indexed yes
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The effect of inter-granular constraints on the response of polycrystalline piezoelectric ceramics at the surface and in the bulk

The electro-mechanical coupling mechanisms in polycrystalline ferroelectric materials, including a soft PbZr₀.₃₅Ti₀.₆₅O₃ (PZT) and lead-free 0.9375(Bi₀.₇Na₀.₃)TiO₃-0.0625BaTiO₃ (BNT-6.25BT), have been studied using a surface sensitive
low-energy (12.4 keV) and bulk sensitive high-energy (73 keV) synchrotron X-ray diffraction with in situ electric fields. The results show that for tetragonal PZT at a maximum electric field of 2.8 kV/mm, the electric-field-induced lattice strain (ε_{111}) is 20% higher at the surface than in the bulk, and non-180° ferroelectric domain texture (as indicated by the intensity ratio I_{002}/I_{200}) is 16% higher at the surface. In the case of BNT-6.25BT, which is pseudo-cubic up to fields of 2 kV/mm, lattice strains, ε_{111} and ε_{200}, are 15% and 20% higher at the surface, while in the mixed tetragonal and rhombohedral phases at 5 kV/mm, the domain texture indicated by the intensity ratio, I_{111}/I_{111} and I_{002}/I_{200}, are 12% and 10% higher at the surface than in the bulk, respectively. The observed difference in the strain contributions between the surface and bulk is suggested to result from the fact that surface grains are not constrained in three dimensions, and consequently, domain reorientation and lattice expansion in surface grains are promoted. It is suggested that the magnitude of property difference between the surface and bulk is higher for the PZT than for BNT-6.25BT due to the level of anisotropy in the strain mechanism. The comparison of the results from different methods demonstrates that the intergranular constraints have a significant influence on the electric-field-induced electro-mechanical responses in polycrystalline ferroelectrics. These results have implications for the design of higher performance polycrystalline piezoelectrics.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, Australian Synchrotron
Authors: Hossain, M. J. (Ekstern), Wang, Z. (Ekstern), Khansur, N. H. (Ekstern), Kimpton, J. A. (Ekstern), Oddershede, J. (Intern), Daniels, J. E. (Ekstern)
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- Scopus rating (2016): CiteScore 2.67 SJR 1.132 SNIP 0.996
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.799 SNIP 1.462 CiteScore 3.25
- Web of Science (2014): Indexed yes
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- Scopus rating (2013): SJR 2.149 SNIP 1.652 CiteScore 3.77
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
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- Scopus rating (2012): SJR 2.554 SNIP 1.754 CiteScore 3.76
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 2.805 SNIP 1.94 CiteScore 4.04
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.926 SNIP 1.789
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
The negative piezoelectric effect of the ferroelectric polymer poly(vinylidene fluoride)

Piezoelectricity describes interconversion between electrical charge and mechanical strain. As expected for lattice ions displaced in an electric field, the proportionality constant is positive for all piezoelectric materials. The exceptions are poly(vinylidene fluoride) (PVDF) and its copolymers with trifluoroethylene (P(VDF-TrFE)), which exhibit a negative longitudinal piezoelectric coefficient. Reported explanations exclusively consider contraction with applied electric field of either the crystalline or the amorphous part of these semi-crystalline polymers. To distinguish between these conflicting interpretations, we have performed in situ dynamic X-ray diffraction measurements on P(VDF-TrFE) capacitors. We find that the piezoelectric effect is dominated by the change in lattice constant but, surprisingly, it cannot be accounted for by the polarization-biased electrostrictive contribution of the crystalline part alone. Our quantitative analysis shows that an additional contribution is operative, which we argue is due to an electromechanical coupling between the intermixed crystalline lamellae and amorphous regions. Our findings tie the counterintuitive negative piezoelectric response of PVDF and its copolymers to the dynamics of their composite microstructure.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Max Planck Institute for Polymer Research, University of Groningen, Swiss Federal Institute of Technology
Pages: 78-84
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Main Research Area: Technical/natural sciences
Thermal decomposition of ammonium hexachloroosmate

Structural changes of (NH₄)₂[OsCl₆] occurring during thermal decomposition in a reduction atmosphere have been studied in situ using combined energy-dispersive X-ray absorption spectroscopy (ED-XAFS) and powder X-ray diffraction (PXRD). According to PXRD, (NH₄)₂[OsCl₆] transforms directly to metallic Os without the formation of any crystalline intermediates but through a plateau where no reactions occur. XANES and EXAFS data by means of Multivariate Curve Resolution (MCR) analysis show that thermal decomposition occurs with the formation of an amorphous intermediate [OsCl₄]ₓ with a possible polymeric structure. Being revealed for the first time the intermediate was subjected to determine the local atomic structure around osmium. The thermal decomposition of hexachloroosmate is much more complex and occurs within a minimum two-step process, which has never been observed before.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, RAS - Nikolaev Institute of Inorganic Chemistry of SB, Novosibirsk State University, Swansea University
Authors: Asanova, T. I. (Ekstern), Kantor, I. (Intern), Asanov, I. P. (Ekstern), Korenev, S. V. (Ekstern), Yusenko, K. V. (Ekstern)
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Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.196
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.127 SNIP 1.369
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
The test beamline of the European Spallation Source - Instrumentation development and wavelength frame multiplication

The European Spallation Source (ESS), scheduled to start operation in 2020, is aiming to deliver the most intense neutron beams for experimental research of any facility worldwide. Its long pulse time structure implies significant differences for instrumentation compared to other spallation sources which, in contrast, are all providing short neutron pulses. In order to enable the development of methods and technology adapted to this novel type of source well in advance of the first instruments being constructed at ESS, a test beamline (TBL) was designed and built at the BER II research reactor at Helmholtz-Zentrum Berlin (HZB). Operating the TBL shall provide valuable experience in order to allow for a smooth start of operations at ESS. The beamline is capable of mimicking the ESS pulse structure by a double chopper system and provides variable wavelength resolution as low as 0.5% over a wide wavelength band between 1.6 Å and 10 Å by a dedicated wavelength frame multiplication (WFM) chopper system. WFM is proposed for several ESS instruments to allow for flexible time-of-flight resolution. Hence, ESS will benefit from the TBL which offers unique possibilities for testing methods and components. This article describes the main capabilities of the instrument, its performance as experimentally verified during the commissioning, and its relevance to currently starting ESS instrumentation projects.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Helmholtz-Zentrum Berlin für Materialien und Energie
Authors: Woracek, R. (Ekstern), Hofmann, T. (Ekstern), Bulat, M. (Ekstern), Sales, M. (Intern), Habicht, K. (Ekstern), Andersen, K. (Ekstern), Strobl, M. (Ekstern)
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Scopus rating (2016): CiteScore 1.44 SJR 0.916 SNIP 1.352
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.915 SNIP 1.334 CiteScore 1.21
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.852 SNIP 1.303 CiteScore 1.24
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.944 SNIP 1.398 CiteScore 1.48
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.806 SNIP 1.071 CiteScore 1.19
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.918 SNIP 1.424 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.893 SNIP 1.113
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.75 SNIP 1.386
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.753 SNIP 1.073
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.716 SNIP 1.383
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.818 SNIP 1.108
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.819 SNIP 1.156
Scopus rating (2004): SJR 0.844 SNIP 1.489
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.673 SNIP 1.226
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.628 SNIP 1.108
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.688 SNIP 1.104
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.594 SNIP 0.974
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Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography

This thesis presents a new technique for measuring spatially resolved microstructures in crystalline materials using pulsed neutron beams. The method, called Time-of-Flight Three Dimensional Neutron Diffraction (ToF 3DND), identifies the position, shape and crystallographic orientation of the individual grains within the sample. The experiments were conducted at the single crystal diffractometer SENJU at the Japanese neutron source J-PARC. The choice of this instrument was motivated by its large coverage of the reciprocal space.

The instrument had to undergo modifications to enable ToF 3DND measurements: a time resolved imaging detector, developed at University of Berkeley, California, was fitted in the interior of SENJU in order to record the extinction spots in the transmitted beam (i.e. areas with missing intensity due to Bragg diffraction of the individual grains).

The arrangement of the two detector systems facilitated two versions of ToF 3DND. The first version, restricted to imaging data, enables reconstruction of the position and shape of the individual grains without the use of crystallography. Afterwards, the orientations of the individual grains are indexed. The algorithms for both steps have been developed in this study. The work also shows that based on the transmission data alone the orientations are not uniquely determined; however, it is possible to find an unique solution by including diffraction signals from the imaging detector. The second version uses an existing method for indexing SENJU data, which then serves as prior information to restrict the extinction spots that belong to the same grain.

The ToF 3DND methods are verified through the study of two different samples: an Iron rod and a shape memory alloy (SMA) CoNiGa bi-crystal. Part of this verification involves comparison with electron backscatter diffraction (EBSD). In the Iron rod, 107 grains were indexed from the SENJU data. As a comparison, 108 grains were reconstructed from the nearfield data alone. This constitutes roughly 10 times as many grains as previously reported using a continuous neutron source.

Thanks to the penetrating properties of the neutron, ToF 3DND complements existing X-ray techniques in those cases where X-rays cannot penetrate the sample. Besides, with ToF 3DND it is also much easier to detect light elements such as those in energy materials.

With a future availability of an energy dispersive x-ray detector with high energy resolution, the methods reported here can be directly transferred to synchrotron and white beam based studies.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Cereser, A. (Intern), Hall, S. A. (Ekstern), Steuwer, A. (Ekstern), Strobl, M. (Ekstern), Schmidt, S. (Intern)
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Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy
Photoexcited Nickel(II) tetramesitylporphyrin (NiTMP), like many open-shell metalloporphyrins, relaxes rapidly through multiple electronic states following an initial porphyrin-based excitation, some involving metal centered electronic configuration changes that could be harnessed catalytically before excited state relaxation. While a NiTMP excited state present at 100 ps was previously identified by X-ray transient absorption (XTA) spectroscopy at a synchrotron source as a relaxed (d,d) state, the lowest energy excited state (J. Am. Chem. Soc., 2007, 129, 9616 and Chem. Sci., 2010, 1, 642), structural dynamics before thermalization were not resolved due to the similar to 100 ps duration of the available X-ray probe pulse. Using the femtosecond (fs) X-ray pulses of the Linac Coherent Light Source (LCLS), the Ni center electronic configuration from the initial excited state to the relaxed (d,d) state has been obtained via ultrafast Ni K-edge XANES (X-ray absorption near edge structure) on a time scale from hundreds of femtoseconds to 100 ps. This enabled the identification of a short-lived Ni(I) species aided by time-dependent density functional theory (TDDFT) methods. Computed electronic and nuclear structure for critical excited electronic states in the relaxation pathway characterize the dependence of the complex's geometry on the electron occupation of the 3d orbitals. Calculated XANES transitions for these excited states assign a short-lived transient signal to the spectroscopic signature of the Ni(I) species, resulting from intramolecular charge transfer on a time scale that has eluded previous synchrotron studies. These combined results enable us to examine the excited state structural dynamics of NiTMP prior to thermal relaxation and to capture intermediates of potential photocatalytic significance.

General information
Uncertainty budget for determinations of mean isomer shift from Mössbauer spectra

The magnetite/maghemite content within iron oxide nanoparticles can be determined using the mean isomer shift (δ¯¯). However, accurate characterisation of the composition is limited by the uncertainty associated with δ¯¯. We have identified four independent sources of uncertainty and developed a quantitative expression for the uncertainty budget. Sources of uncertainty are categorised as follows: that from the fitting of the Mössbauer spectrum (σfit), that of the calibration of the α-Fe reference spectrum (σcal), thermal corrections to the spectrum due to second order Doppler shift (SODS) (σΔδ) and other experimental errors (σerr). Each contribution is discussed in detail using 57Fe Mössbauer spectra obtained from an iron oxide nanoparticle system at temperatures between 16 K and 295 K on different spectrometers in two different laboratories.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Physikalisch-Technische Bundesanstalt, University College London
Authors: Fock, J. (Intern), Bogart, L. K. (Ekstern), Posth, O. (Ekstern), Hansen, M. F. (Intern), Pankhurst, Q. A. (Ekstern), Frandsen, C. (Intern)
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Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
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Universal amorphous-amorphous transition in $\text{Ge}_{x}\text{Se}_{100-x}$ glasses under pressure

Pressure induced structural modifications in vitreous $\text{GeXSe}_{100-x}$ (where $10 \leq x \leq 25$) are investigated using X-ray absorption spectroscopy (XAS) along with supplementary X-ray diffraction (XRD) experiments and ab initio molecular dynamics (AIMD) simulations. Universal changes in distances and angle distributions are observed when scaled to reduced densities. All compositions are observed to remain amorphous under pressure values up to 42 GPa. The Ge-Se interatomic distances extracted from XAS data show a two-step response to the applied pressure; a gradual decrease followed by an increase at around 15–20 GPa, depending on the composition. This increase is attributed to the metallization event that can be traced with the red shift in Ge K edge energy which is also identified by the principal peak position of the structure factor. The densification mechanisms are studied in details by means of AIMD simulations and compared to the experimental results. The evolution of bond angle distributions, interatomic distances and coordination numbers are examined and lead to similar pressure-induced structural changes for any composition.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Universite de Liege, Sorbonne Universités, University of Cincinnati, European Synchrotron Radiation Facility, Ehime University
Authors: Yildirim, C. (Ekstern), Micoulaut, M. (Ekstern), Boolchand, P. (Ekstern), Kantor, I. (Intern), Mathon, O. (Ekstern), Gaspard, J. (Ekstern), Irifune, T. (Ekstern), Raty, J. (Ekstern)
Water-Mediated Ion Pairing: Occurrence and Relevance

We present an overview of the studies of ion pairing in aqueous media of the past decade. In these studies, interactions between ions, and between ions and water, are investigated with relatively novel approaches, including dielectric relaxation spectroscopy, far-infrared (terahertz) absorption spectroscopy, femtosecond mid-infrared spectroscopy, and X-ray spectroscopy and scattering, as well as molecular dynamics simulation methods. With these methods, it is found that ion pairing is not a rare phenomenon only occurring for very particular, strongly interacting cations and anions. Instead, for many salt solutions and their interfaces, the measured and calculated structure and dynamics reveal the presence of a distinct concentration of contact ion pairs (CIPs), solvent shared ion pairs (SIPs), and solvent-separated ion pairs (2SIPs). We discuss the importance of specific ion-pairing interactions between cations like Li(+) and Na(+) and anionic carboxylate and phosphate groups for the structure and functioning of large (bio)molecular systems.

General information
A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Iron(II)

Strongly sigma-donating N-heterocyclic carbenes (NHCs) have revived research interest in the catalytic chemistry of iron, and are now also starting to bring the photochemistry and photophysics of this abundant element into a new era. In this work, a heteroleptic Fe-II complex (1) was synthesized based on sequentially furnishing the Fe-II center with the benchmark 2,2-bipyridine (bpy) ligand and the more strongly sigma-donating mesoionic ligand, 4,4-bis(1,2,3-triazol-5-ylidene) (btz). Complex1 was comprehensively characterized by electrochemistry, static and ultrafast spectroscopy, and quantum chemical calculations and compared to [Fe(bpy)(3)][PF6](2) and (TBA)(2)[Fe(bpy)(CN)(4)]. Heteroleptic complex1 extends the absorption spectrum towards longer wavelengths compared to a previously synthesized homoleptic Fe-II NHC complex. The combination of the mesoionic nature of btz and the heteroleptic structure effectively destabilizes the metal-centered (MC) states relative to the triplet metal-to-ligand charge transfer ((MLCT)-M-3) state in 1, rendering it a
lifetime of 13ps, the longest to date of a photochemically stable Fe-II complex. Deactivation of the (MLCT)-M-3 state is proposed to proceed via the (MC)-M-3 state that strongly couples with the singlet ground state.

**General information**
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Lund University, Uppsala University
Authors: Liu, Y. (Ekstern), Kjær, K. S. (Intern), Fredin, L. A. (Ekstern), Chabera, P. (Ekstern), Harlang, T. C. B. (Ekstern), Canton, S. E. (Ekstern), Lidin, S. (Ekstern), Zhang, J. (Ekstern), Lomoth, R. (Ekstern), Bergquist, K. (Ekstern), Persson, P. (Ekstern), Wärnmark, K. (Ekstern), Sundström, V. (Ekstern)
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Web of Science (2017): Indexed yes
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
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Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 2.527 SNIP 1.292
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.499 SNIP 1.365
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.887 SNIP 1.407
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.233 SNIP 1.532
Scopus rating (2006): SJR 2.911 SNIP 1.505
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.62 SNIP 1.454
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
Authors: Winther, G. (Intern), Oddershede, J. (Intern), Wright, J. (Ekstern)
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Relations
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Projects:
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity
Publication: Research › Conference abstract for conference – Annual report year: 2015

Analysis of the crystallographic and magnetic structures of the $\text{Tb}_{0.1}\text{Pr}_{0.9}\text{Al}_2$ and $\text{Tb}_{0.25}\text{Pr}_{0.75}\text{Al}_2$ magnetocaloric compounds by means of neutron scattering
Neutron powder diffraction and inelastic neutron scattering data were used to simulate and understand the magnetization and heat capacity curves of the pseudobinary $\text{Tb}_x\text{Pr}_{1-x}\text{Al}_2$, with $x = 0.10$ and 0.25, as a function of temperature. From the Rietveld analysis, we concluded that no crystallographic transition occurs in these samples, and the high symmetry of the magnetic structure was confirmed. Moreover, the different contributions from the reflection planes could be related to the known exchange bias-like effect characteristic for the $x = 0.25$ sample, also suggesting the existence of some rearrangement of the magnetic moments or even the presence of spin frustration in this system. Finally, the obtained set of theoretical parameters using the mean field approach for the two systems consisting of two sublattices allowed the experimental data to be described and to explain their physical behaviors. The ensemble of our results leads us to affirm that the quadrupolar interactions as well as an existence of some rearrangement of the magnetic moments or a frustration play an important role in the strong unidirectional anisotropy and the exchange bias-like effect observed in this pseudobinary system.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Brazilian Synchrotron Light Laboratory, Rutherford Appleton Laboratory, Helmholtz-Zentrum Berlin für Materialien und Energie,
Anomalous magnetic structure and spin dynamics in magnetoelectric LiFePO$_4$

Anomalous magnetic structure and spin dynamics in magnetoelectric LiFePO$_4$ obtained by single-crystal neutron scattering. Our results confirm a previously reported collinear rotation of the spins away from the principal b axis, and they determine that the rotation is toward the a axis. In addition, we find a significant spin-canting component along c. The possible causes of these components are discussed, and their significance for the magnetoelectric effect is analyzed. Inelastic neutron scattering along the three principal directions reveals a highly anisotropic hard plane consistent with earlier susceptibility measurements. Using a spin Hamiltonian, we show that the spin dimensionality is intermediate between XY- and Ising-like, with an easy b axis and a hard c axis. It is shown that both next-nearest neighbor exchange couplings in the bc plane are in competition with the strongest nearest neighbor coupling.
By use of Mossbauer spectroscopy we have studied the magnetic properties of samples of goethite nanoparticles with different particle size. The spectra are influenced by fluctuations of the magnetization directions, but the size dependence is not in accordance with the Neel-Brown expression for superparamagnetic relaxation of the magnetization vectors of the particles as a whole. The data suggest that the magnetic fluctuations can be explained by fluctuations of the magnetization directions of small interacting grains within the particles.
Application of Generalized Mie Theory to EELS Calculations as a Tool for Optimization of Plasmonic Structures

Technical applications of plasmonic nanostructures require a careful structural optimization with respect to the desired functionality. The success of such optimizations strongly depends on the applied method. We extend the generalized multiparticle Mie (GMM) computational electromagnetic method and use it to excite a system of plasmonic nanoparticles with an electron beam. This method is applied to EELS calculations of a gold dimer and compared to other methods. It is demonstrated that the GMM method is so efficient, that it can be used in the context of structural optimization by the application of genetic algorithms combined with a simplex algorithm. The scheme is applied to the design of plasmonic filters.
Broad spectrum moderators and advanced reflector filters using $^{208}$Pb

Cold and thermal neutrons used in neutrons scattering experiments are produced in nuclear reactors and spallation sources. The neutrons are cooled to thermal or cold temperatures in thermal and cold moderators, respectively. The present study shows that it is possible to exploit the poor thermalizing property of $^{208}$Pb to design a broad spectrum moderator, i.e. a moderator which emits thermal and cold neutrons from the same position. Using $^{208}$Pb as a reflector filter material is shown to be slightly less efficient than a conventional beryllium reflector filter. However, when surrounding the reflector filter by a cold moderator it is possible to regain the neutrons with wavelengths below the Bragg edge, which are suppressed in the beryllium reflector filter. In both the beryllium and lead case surrounding the reflector filter with a cold moderator increases the cold brightness significantly compared to a conventional reflector filter.

Keywords
Mie theory, Optimization, Electron energy loss spectroscopy
Characterization of nano-textured samples in a production environment

Nano-textured surfaces have been characterized by optical diffraction techniques using an adapted commercial light microscope with two detectors, a CCD camera and a spectrometer. We demonstrate that the microscope has a resolution in the nanometer range, also in an environment with many vibrations, such as a machine floor. The acquisition and analysing time for the topological parameters height, width and sidewall angle is only a few milliseconds.

It is demonstrated that by simple adaptions to an optical microscope we can measure nano-textured surfaces with an uncertainty of a few nanometers for the height and width of the structures. The microscope has been validated by measuring on certified transfer artefact and 1D gratings. The measurements are very robust, such that vibrations of the sample and/or the microscope do not affect the results. The sample can be translated during acquisition, as long as the beam spot is kept inside an area with homogenous structures, which makes the proposed microscope well suited for implementation in a production environment.

Competing superconducting and magnetic order parameters and field-induced magnetism in electron doped Ba(Fe_{1-x}Co_{x})_{2}As_{2}

We have studied the magnetic and superconducting properties of Ba(Fe_{1-x}Co_{x})_{2}As_{2} as a function of temperature and external magnetic field using neutron scattering and muon spin rotation. Below the superconducting transition temperature the magnetic and superconducting order parameters coexist and compete. A magnetic field can significantly enhance the magnetic scattering in the superconducting state, roughly doubling the Bragg intensity at 13.5 T. We perform a microscopic modelling of the data by use of a five-band Hamiltonian relevant to iron pnictides. In the superconducting state, vortices can slow down and freeze spin fluctuations locally. When such regions couple they result in a long-range ordered antiferromagnetic phase producing the enhanced magnetic elastic scattering in agreement with experiments.
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Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.982 SNIP 1.524
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.923 SNIP 1.546
Web of Science (2007): Indexed yes
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Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.763 SNIP 1.607
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.742 SNIP 1.606
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.75 SNIP 1.536
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.788 SNIP 1.706
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.946 SNIP 1.635
Web of Science (2001): Indexed yes
Composite Microdiscs with a Magnetic Belt: Preparation, Chaining Properties, and Use as Switchable Catalyst Carriers

We describe an emulsion-based preparation of patchy composite particles (diameter of 100-500 μm) consisting of a disclike epoxy core and a belt of porous polystyrene particles (diameter of 30 μm) with magnetite within the pores. Compared to the magnetically uniform polystyrene particles, the spontaneous aggregation of composite particles is suppressed when dispersed into liquid, which is attributed to the increased particle size, reduced magnetic susceptibility, and the shape of the magnetic domain distribution within the particles (spherical versus a belt). When the composite particles are coated by platinum-palladium layer we demonstrate they can be employed as switchable catalyst carriers, moving from one liquid phase to another when controlled by an external magnetic field.
Correction of complex nonlinear signal response from a pixel array detector

The pulsed free-electron laser light sources represent a new challenge to photon area detectors due to the intrinsic spontaneous X-ray photon generation process that makes single-pulse detection necessary. Intensity fluctuations up to 100% between individual pulses lead to high linearity requirements in order to distinguish small signal changes. In real detectors, signal distortions as a function of the intensity distribution on the entire detector can occur. Here a robust method to correct this nonlinear response in an area detector is presented for the case of exposures to similar signals. The method is tested for the case of diffuse scattering from liquids where relevant sub-1% signal changes appear on the same order as artifacts induced by the detector electronics.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory
Authors: Brandt van Driel, T. (Intern), Herrmann, S. (Ekstern), Carini, G. (Ekstern), Nielsen, M. M. (Intern), Lemke, H. T. (Ekstern)
Number of pages: 8
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Scopus rating (2016): CiteScore 2.86 SJR 1.593 SNIP 1.578
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.161 SNIP 1.396 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.505 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.473 SNIP 1.687 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.558 SNIP 1.273 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
Dark-field X-ray microscopy for multiscale structural characterization

Many physical and mechanical properties of crystalline materials depend strongly on their internal structure, which is typically organized into grains and domains on several length scales. Here we present dark-field X-ray microscopy, a non-destructive microscopy technique for the three-dimensional mapping of orientations and stresses on lengths scales from 100 nm to 1 mm within embedded sampling volumes. The technique, which allows ‘zooming’ in and out in both direct and angular space, is demonstrated by an annealing study of plastically deformed aluminium. Facilitating the direct study of the interactions between crystalline elements is a key step towards the formulation and validation of multiscale models that account for the entire heterogeneity of a material. Furthermore, dark-field X-ray microscopy is well suited to applied topics, where the structural evolution of internal nanoscale elements (for example, positioned at interfaces) is crucial to the performance and lifetime of macro-scale devices and components thereof.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Mechanical Engineering, Materials and Surface Engineering, DTU Danchip, European Synchrotron Radiation Facility, Institut National des Sciences Appliquées de Lyon
Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Communications
Volume: 6
Dark field X-ray microscopy for studies of recrystallization

We present the recently developed technique of Dark Field X-Ray Microscopy that utilizes the diffraction of hard X-rays from individual grains or subgrains at the (sub)micrometre-scale embedded within mm-sized samples. By magnifying the diffracted signal, 3D mapping of orientations and strains inside the selected grain is performed with an angular resolution of 0.005° and a spatial resolution of 200 nm. Furthermore, the speed of the measurements at high-intensity synchrotron facilities allows for fast non-destructive in situ determination of structural changes induced by annealing or other external influences. The capabilities of Dark Field X-Ray Microscopy are illustrated by examples from an ongoing study of recrystallization of 50% cold-rolled Al1050 specimens.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Wind Energy, Materials science and characterization, DTU Danchip
Number of pages: 7
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Deformation-induced orientation spread in individual bulk grains of an interstitial-free steel

Three-dimensional X-ray diffraction was employed to characterize the lattice rotations of individual bulk grains in a 9% tensile deformed sample of interstitial-free steel. Three grains of initially close orientation that are representative of the scatter of all investigated grains with tensile axes near <522> were identified. Their rotation paths and intragranular orientation spread were analysed in detail, using crystal plasticity modelling to evaluate the nature of the orientation spread. It was found that the same set of most stressed slip systems are active in the three grains and that variations in the relative activities of the two most stressed systems account for the dominant orientation spread in the grains. The distribution of slip on these systems varies from grain to grain and also within each grain. While the grain orientation controls the identity of these slip systems, the variations are attributed to grain boundary and grain interaction effects. © 2014 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 5.67 SJR 3.283 SNIP 2.674
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 3.542 SNIP 2.927 CiteScore 5.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 4.045 SNIP 3.348 CiteScore 5.16
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 3.29 SNIP 2.709 CiteScore 4.37
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.409 SNIP 2.917 CiteScore 4.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.247 SNIP 2.81 CiteScore 4.27
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.745 SNIP 2.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.677 SNIP 2.648
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.863 SNIP 2.787
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.298 SNIP 3.068
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.172 SNIP 3.082
Scopus rating (2004): SJR 3.066 SNIP 3.154
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 4.016 SNIP 3.081
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.225 SNIP 2.732
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.706 SNIP 2.194
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.188 SNIP 2.177

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Ferritic steels, Tensile behaviour, High-energy X-ray diffraction, Individual bulk grains, Crystal plasticity
Electronic versions:
Theoretical predictions show that depending on the populations of the Fe 3d(xy), 3d(xz), and 3d(yz) orbitals two possible quintet states can exist for the high-spin state of the photoswitchable model system \([\text{Fe(terpy)}(2)^{2+}]\). The differences in the structure and molecular properties of these B-5(2) and E-5 quintets are very small and pose a substantial challenge for experiments to resolve them. Yet for a better understanding of the physics of this system, which can lead to the design of novel molecules with enhanced photoswitching performance, it is vital to determine which high-spin state is reached in the transitions that follow the light excitation. The quintet state can be prepared with a short laser pulse and can be studied with cutting-edge time-resolved X-ray techniques. Here we report on the application of an extended set of X-ray spectroscopy and scattering techniques applied to investigate the quintet state of \([\text{Fe(terpy)}(2)^{2+}]\) 80 ps after light excitation. High-quality X-ray absorption, nonresonant emission, and resonant emission spectra as well as X-ray diffuse scattering data clearly reflect the formation of the high-spin state of the \([\text{Fe(terpy)}(2)^{2+}]\) molecule; moreover, extended X-ray absorption fine structure spectroscopy resolves the Fe-ligand bond-length variations with unprecedented bond-length accuracy in time-resolved experiments. With ab initio calculations we determine why, in contrast to most related systems, one configurational mode is insufficient for the description of the low-spin (LS)-high-spin (HS) transition. We identify the electronic structure origin of the differences between the two possible quintet modes, and finally, we unambiguously identify the formed quintet state as 5E, in agreement with our theoretical expectations.
With the arrival of X-ray Free Electron Lasers (XFELs), 2D area detectors with a large dynamic range for detection of hard X-rays with fast readout rates are required for many types of experiments. Extracting the desired information from these detectors has been challenging due to unpredicted fluctuations in the measured images. For techniques such as time-resolved X-ray Diffuse Scattering (XDS), small differences in signal intensity are the starting point for analysis. Fluctuations in the total detected signal remain in the differences under investigation, obfuscating the signal. To correct such artefacts, Singular Value Decomposition (SVD) can be used to identify and characterize the observed detector fluctuations and assist in assigning some of them to variations in physical parameters such as X-ray energy and X-ray intensity. This paper presents a methodology for robustly identifying, separating and correcting fluctuations on area detectors based on XFEL beam characteristics, to enable the study of temporally resolved solution state chemistry on the femtosecond timescale.

**Disentangling detector data in XFEL studies of temporally resolved solution state chemistry**

With the arrival of X-ray Free Electron Lasers (XFELs), 2D area detectors with a large dynamic range for detection of hard X-rays with fast readout rates are required for many types of experiments. Extracting the desired information from these detectors has been challenging due to unpredicted fluctuations in the measured images. For techniques such as time-resolved X-ray Diffuse Scattering (XDS), small differences in signal intensity are the starting point for analysis. Fluctuations in the total detected signal remain in the differences under investigation, obfuscating the signal. To correct such artefacts, Singular Value Decomposition (SVD) can be used to identify and characterize the observed detector fluctuations and assist in assigning some of them to variations in physical parameters such as X-ray energy and X-ray intensity. This paper presents a methodology for robustly identifying, separating and correcting fluctuations on area detectors based on XFEL beam characteristics, to enable the study of temporally resolved solution state chemistry on the femtosecond timescale.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory
Double-slit experiment with single wave-driven particles and its relation to quantum mechanics

In a thought-provoking paper, Couder and Fort [Phys. Rev. Lett. 97, 154101 (2006)] describe a version of the famous double-slit experiment performed with droplets bouncing on a vertically vibrated fluid surface. In the experiment, an interference pattern in the single-particle statistics is found even though it is possible to determine unambiguously which slit the walking droplet passes. Here we argue, however, that the single-particle statistics in such an experiment will be fundamentally different from the single-particle statistics of quantum mechanics. Quantum mechanical interference takes place between different classical paths with precise amplitude and phase relations. In the double-slit experiment with walking droplets, these relations are lost since one of the paths is singled out by the droplet. To support our conclusions, we have carried out our own double-slit experiment, and our results, in particular the long and variable slit passage times of the droplets, cast strong doubt on the feasibility of the interference claimed by Couder and Fort. To understand theoretically the limitations of wave-driven particle systems as analogs to quantum mechanics, we introduce a Schrödinger equation with a source term originating from a localized particle that generates a wave while being simultaneously guided by it. We show that the ensuing particle-wave dynamics can capture some characteristics of quantum mechanics such as orbital quantization. However, the particle-wave dynamics cannot reproduce quantum mechanics in general, and we show that the single-particle statistics for our model in a double-slit experiment with an additional splitter plate differs qualitatively from that of quantum mechanics.
Dynamics of chemical bond: general discussion

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.7 SNIP 1.278 CiteScore 3.79
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Scopus rating (2013): SJR 1.618 SNIP 1.12 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 0.948 CiteScore 3.24
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.893 SNIP 1.239 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.719 SNIP 1.22
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.799 SNIP 1.157
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.792 SNIP 1.293
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.898 SNIP 1.316
Scopus rating (2006): SJR 1.39 SNIP 1.148
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.32 SNIP 0.986
Scopus rating (2004): SJR 0.994 SNIP 0.885
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.029 SNIP 0.868
Scopus rating (2002): SJR 1.124 SNIP 0.847
Scopus rating (2001): SJR 1.249 SNIP 0.655
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.109 SNIP 0.806
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.925 SNIP 0.734
Original language: English
Chemistry, Enhanced raman-spectroscopy
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Bibliographical note
Discussion summary from one of more discussion meetings that focus on rapidly developing areas of chemistry.
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Publication: Research - peer-review › Journal article – Annual report year: 2015

Effect of maghemization on the magnetic properties of pseudo-single-domain magnetite particles

General information
Electron Injection from Copper Diimine Sensitizers into TiO2: Structural Effects and Their Implications for Solar Energy Conversion Devices

Copper(I) diimine complexes have emerged as low cost replacements for ruthenium complexes as light sensitizers and electron donors, but their shorter metal-to-ligand-charge-transfer (MLCT) states lifetimes and lability of transient Cu(II) species impede their intended functions. Two carboxylated Cu(I) bis-2,9-diphenylphenanthroline (dpp) complexes [Cu(I)(dpp-O(CH2CH2O)5)(dpp-(COOH)2)]+ and [Cu(I)(dpp-O(CH2CH2O)5)(dpp-(Φ-COOH)2)]+ (Φ = tolyl) with different linker lengths were synthesized in which the MLCT-state solvent quenching pathways are effectively blocked, the lifetime of the singlet MLCT state is prolonged, and the transient Cu(II) ligands are stabilized. Aiming at understanding the mechanisms of structural influence to the interfacial charge transfer in the dye-sensitized solar cell mimics, electronic and geometric structures as well as dynamics for the MLCT state of these complexes and their hybrid with TiO2 nanoparticles were investigated using optical transient spectroscopy, X-ray transient absorption spectroscopy, time-dependent density functional theory, and quantum dynamics simulations. The combined results show that these complexes exhibit strong absorption throughout the visible spectrum due to the severely flattened ground state, and a long-lived charge-separated Cu(II) has been achieved via ultrafast electron injection (<300 fs) from the MLCT state into TiO2 nanoparticles. The results also indicate that the TiO2-phen distance in these systems does not have significant effect on the efficiency of the interfacial electron-transfer process. The mechanisms for electron transfer in these systems are discussed and used to develop new strategies in optimizing copper(I) diimine complexes in solar energy conversion devices.
Fast Characterization of Moving Samples with Nano-Textured Surfaces

Characterization of structures using conventional optical microscopy is restricted by the diffraction limit. Techniques like atomic force and scanning electron microscopy can investigate smaller structures but are very time consuming. We show that using scatterometry, a technique based on optical diffraction, integrated into a commercial light microscope we can characterize nano-textured surfaces in a few milliseconds. The adapted microscope has two detectors, a CCD camera used to easily find an area of interest and a spectrometer for the measurements. We demonstrate that the microscope has a resolution in the nanometer range for the topographic parameters: height, width, and sidewall angle of a periodic grating, also in an environment with many vibrations, such as a production facility with heavy equipment.

Field-induced interplanar magnetic correlations in the high-temperature superconductor La$_{1.88}$Sr$_{0.12}$CuO$_4$

We present neutron-scattering studies of the interplanar magnetic correlations in the high-temperature superconductor La$_{1.88}$Sr$_{0.12}$CuO$_4$ ($T_c=27$ K). The correlations are studied both in a magnetic field applied perpendicular to the CuO$_2$ planes, and in zero field under different cooling conditions. We find that the effect of the magnetic field is to increase the magnetic scattering signal at all values of the out-of-plane wave vector $L$, indicating an overall increase of the magnetic moments. In addition, weak correlations between the copper oxide planes develop in the presence of a magnetic field. This effect is not taken into account in previous reports on the field effect of magnetic scattering, since usually only $L=0$ is probed. Interestingly, the results of quench-cooling the sample are similar to those obtained by applying a magnetic field. Finally, a small variation of the incommensurate peak position as a function of $L$ provides evidence that the incommensurate signal is twinned with the magnetic scattering from the dominant and subdominant structural twin.
displaying peaks at even and odd values of L, respectively, in our crystal.

**General information**

State: Published

Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Paul Scherrer Institut, Heinz Maier-Leibnitz-Zentrum, Hokkaido University, Muroran Institute of Technology, Research Centre Julich (FZJ), Helmholtz–Zentrum Berlin für Materialien und Energie


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Publication date: 2015

Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 3.16

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BFI (2015): BFI-level 2

Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 2

Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 2

Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

BFI (2012): BFI-level 2

Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 2

Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61

ISI indexed (2011): ISI indexed yes

Web of Science (2011): Indexed yes

BFI (2010): BFI-level 2

Scopus rating (2010): SJR 3.417 SNIP 1.451

Web of Science (2010): Indexed yes

BFI (2009): BFI-level 2

Scopus rating (2009): SJR 3.109 SNIP 1.474

Web of Science (2009): Indexed yes

BFI (2008): BFI-level 1

Scopus rating (2008): SJR 2.982 SNIP 1.524

Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 2.923 SNIP 1.546

Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 2.796 SNIP 1.56

Web of Science (2006): Indexed yes
Formation and transformation of a short range ordered iron carbonate precursor

Fe(II)-carbonates, such as siderite, form in environments where O₂ is scarce, e.g., during marine sediment diagenesis, corrosion and possibly CO₂ sequestration, but little is known about their formation pathways. We show that early precipitates from carbonate solutions containing 0.1M Fe(II) with varying pH produced broad peaks in X-ray diffraction and contained dominantly Fe and CO₃ when probed with X-ray photoelectron spectroscopy. Reduced pair distribution function (PDF) analysis shows only peaks corresponding to interatomic distances below 15Å, reflecting a material with no long range structural order. Moreover, PDF peak positions differ from those for known iron carbonates and hydroxides. Mössbauer spectra also deviate from those expected for known iron carbonates and suggest a less crystalline structure. These data show that a previously unidentified iron carbonate precursor phase formed. Its coherent scattering domains determined from PDF analysis are slightly larger than for amorphous calcium carbonate, suggesting that the precursor could be nanocrystalline. Replica exchange molecular dynamics simulations of Fe-carbonate polynuclear complexes yield PDF peak positions that agree well with those from experiments, offering the possibility that the material is a condensate of such complexes, assembled in a relatively unorganised fashion. If this is the case, the material could be nearly amorphous, rather than being composed of well defined nanocrystals. PDF measurements of samples ageing in solution coupled with refinement with the software PDFgui show that the material transforms to siderite or siderite/chukanovite mixtures within hours and that the transformation rate depends on pH. The identified Fe-carbonate precursor may potentially form during anaerobic corrosion or bacterial Fe reduction.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, University of Delaware, Université Pierre et Marie Curie, University of California, Pacific Northwest National Laboratory
Authors: Dideriksen, K. (Ekstern), Frandsen, C. (Intern), Bovet, N. (Ekstern), Wallace, A. F. (Ekstern), Sel, O. (Ekstern), Arbour, T. (Ekstern), Navrotsky, A. (Ekstern), De Yoreo, J. J. (Ekstern), Banfield, J. F. (Ekstern)
Number of pages: 16
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Main Research Area: Technical/natural sciences

Publication information
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Volume: 164
ISSN (Print): 0016-7037
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Quantum magnets have occupied the fertile ground between many-body theory and low-temperature experiments on real materials since the early days of quantum mechanics. However, our understanding of even deceptively simple systems of interacting spin-1/2 particles is far from complete. The quantum square-lattice Heisenberg antiferromagnet, for example, exhibits a striking anomaly of hitherto unknown origin in its magnetic excitation spectrum. This quantum effect manifests itself for excitations propagating with the specific wavevector \((\pi,0)\). We use polarized neutron spectroscopy to fully characterize the magnetic fluctuations in the metal-organic compound \(\text{Cu(DCOO)}_2 \cdot 4\text{H}_2\text{O}\), a known realization of the quantum square-lattice Heisenberg antiferromagnet model. Our experiments reveal an isotropic excitation continuum at the anomaly, which we analyse theoretically using Gutzwiller-projected trial wavefunctions. The excitation continuum is accounted for by the existence of spatially extended pairs of fractional \(S=1/2\) quasiparticles, 2D analogues of 1D spinons. Away from the anomalous wavevector, these fractional excitations are bound and form conventional magnons. Our results establish the existence of fractional quasiparticles in the high-energy spectrum of a quasi-two-dimensional antiferromagnet, even in the absence of frustration.

**Fractional excitations in the square-lattice quantum antiferromagnet**

Quantum magnets have occupied the fertile ground between many-body theory and low-temperature experiments on real materials since the early days of quantum mechanics. However, our understanding of even deceptively simple systems of interacting spin-1/2 particles is far from complete. The quantum square-lattice Heisenberg antiferromagnet, for example, exhibits a striking anomaly of hitherto unknown origin in its magnetic excitation spectrum. This quantum effect manifests itself for excitations propagating with the specific wavevector \((\pi,0)\). We use polarized neutron spectroscopy to fully characterize the magnetic fluctuations in the metal-organic compound \(\text{Cu(DCOO)}_2 \cdot 4\text{H}_2\text{O}\), a known realization of the quantum square-lattice Heisenberg antiferromagnet model. Our experiments reveal an isotropic excitation continuum at the anomaly, which we analyse theoretically using Gutzwiller-projected trial wavefunctions. The excitation continuum is accounted for by the existence of spatially extended pairs of fractional \(S=1/2\) quasiparticles, 2D analogues of 1D spinons. Away from the anomalous wavevector, these fractional excitations are bound and form conventional magnons. Our results establish the existence of fractional quasiparticles in the high-energy spectrum of a quasi-two-dimensional antiferromagnet, even in the absence of frustration.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Johns Hopkins University, University of Edinburgh, Paul Scherrer Institut, Institut Max von Laue-Paul
Results based on virtual instrument models for the first high-flux, high-resolution, spallation based, backscattering spectrometer, BASIS are presented in this paper. These were verified using the Monte Carlo instrument simulation packages McStas and VITESS. Excellent agreement of the neutron count rate at the sample position between the virtual instrument simulation and experiments was found, in both time and energy distributions. This achievement was only possible after a new component for a bent single crystal analyser in McStas, using a Gaussian approximation, was developed. These findings are pivotal to the conceptual design of the next generation backscattering spectrometer, MIRACLES at the European Spallation Source.
Generalized balanced power diagrams for 3D representations of polycrystals

Characterizing the grain structure of polycrystalline material is an important task in material science. The present paper introduces the concept of generalized balanced power diagrams as a concise alternative to voxelated mappings. Here,
each grain is represented by (measured approximations of) its centre of mass position, its volume and, if available, and by
its second-order moments (in the non-equiaxed case). Such parameters may be obtained from 3D X-ray diffraction. As the
exact global optimum of our model results from the solution of a suitable linear programme it can be computed quite
efficiently. Based on verified real-world measurements, we show that from the few parameters per grain (3, respectively, 6
in 2D and 4, respectively, 10 in 3D) we obtain excellent representations of both equiaxed and non-equiaxed structures.
Hence our approach seems to capture the physical principles governing the forming of such polycrystals in the underlying
process quite well.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technische Universität München,
Universität der Bundeswehr München, Xnovo Technology ApS
Authors: Alpers, A. (Ekstern), Brieden, A. (Ekstern), Gritzmann, P. (Ekstern), Lyckegaard, A. (Ekstern), Poulsen, H. F.
(Intern)
Pages: 1016-1028
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Main Research Area: Technical/natural sciences

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Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.34 SJR 0.735 SNIP 0.714
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.888 SNIP 0.985 CiteScore 1.52
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.957 SNIP 1.11 CiteScore 1.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.902 SNIP 0.936 CiteScore 1.46
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.013 SNIP 0.953 CiteScore 1.45
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.933 SNIP 0.976 CiteScore 1.43
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.034 SNIP 0.959
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.06 SNIP 0.853
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.231 SNIP 0.996
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.113 SNIP 1.081
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.184 SNIP 1.152
Web of Science (2006): Indexed yes
High-\(J_c\) \(\text{YBa}_2\text{Cu}_3\text{O}_7\text{-Ag}\) superconducting thin films synthesized through a fluorine-free MOD method

Obtaining a high critical current density (\(J_c\)) remains the main challenge in developing fluorine-free metal organic deposition (MOD) methods to fabricate YBCO superconducting thin films. Silver addition was used to raise the \(J_c\) values in this research work. By reacting with propionic acid and ammonia, \(\text{AgNO}_3\) was initially mixed with YBCO carboxylate precursors dissolved in methanol. High-temperature in situ XRD measurements on the YBCO-Ag powders revealed that silver addition lowers the incongruent melting temperature of YBCO to 760°C and resulted in a smooth surface morphology of the YBCO films at a temperature as low as 760°C. Grain growth and intergranular conductivity were also found to be improved by silver doping. After annealing under optimized conditions, a high \(J_c\) of 4.6MA/cm² was obtained in a YBCO-Ag thin film with 10 wt% Ag.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Tsinghua University
Authors: Tang, X. (Intern), Yue, Z. (Intern), Wu, W. (Ekstern), Grivel, J. (Intern), Andersen, N. H. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 3.25 SJR 1.135 SNIP 1.776
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.15 SNIP 1.841 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.187 SNIP 2.099 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.122 SNIP 1.794 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 2.244 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Injection molded polymeric hard X-ray lenses

A novel and economical approach for fabricating compound refractive lenses for the purpose of focusing hard X-rays is described. A silicon master was manufactured by UV-lithography and deep reactive ion etching (DRIE). Sacrificial structures were utilized, which enabled accurate control of the etching profile and were removed after DRIE. By electroplating, an inverse nickel sample was obtained, which was used as a mold insert in a commercial polymer injection molding machine. A prototype lens made of polyethylene with a focal length of 350 mm was tested using synchrotron radiation at photon energies of 17 keV. A 55 µm long line focus with a minimal waist of 770 nm (FWHM) and a total lens transmittance of 32% were measured. Due to its suitability for cheap mass production, this highly efficient optics may find widespread use in hard X-ray instruments.

General information
State: Published
Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Pages: 2804-2811
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Main Research Area: Technical/natural sciences

Publication information
Journal: Optical Materials Express
Volume: 5
In Situ Studies of Fe\(^{4+}\) Stability in β-Li3Fe2(PO4)3 Cathodes for Li Ion Batteries

In commercial Fe-based batteries the Fe\(^{2+}/Fe^{3+}\) oxidation states are used, however by also utilizing the Fe\(^{4+}\) oxidation state, intercalation of up to two Li ions per Fe ion could be possible. In this study, we investigate whether Fe\(^{4+}\) can be formed and stabilized in β-Li3Fe2(PO4)3. The work includes in situ synchrotron X-ray powder diffraction studies (XRPD) during charging of β-Li3Fe2(PO4)3 up to 5.0 V vs. Li/Li+. A novel capillary-based micro battery cell for in situ XRPD has been designed for this. During charge, a plateau at 4.5 V was found and a small contraction in volume was observed, indicating some Li ion extraction. The volume change of the rhombohedral unit cell is anisotropic, with a decrease in the a parameter and an increase in the c parameter during the Li ion extraction. Unfortunately, no increased discharge capacity was observed and Mössbauer spectroscopy showed no evidence of Fe\(^{4+}\) formation. Oxidation of the organic electrolyte is inevitable at 4.5 V but this alone cannot explain the volume change. Instead, a reversible oxygen redox process (O\(^2−\) → O\(^−\)) could possibly explain and charge compensate for the reversible extraction of lithium ions from β-Li3Fe2(PO4)3.
Bibliographical note
Erratum in Electrochemical Society. Journal, 2015, 162(6) p. X11: Throughout this paper, the prefix “β-” has been used incorrectly to indicate the rhombohedral phase of Li3Fe2(PO4)3. The material studied in the paper is exclusively the rhombohedral phase and all instances of “β-Li3Fe2(PO4)3” should be replaced with “Li3Fe2(PO4)3.”

Source: FindIt
Interactions of a zwitterionic thiophene-based conjugated polymer with surfactants

In this paper we investigate the optical and structural properties of a zwitterionic poly[3-(N-(4-sulfonato-1-butyl)-N,N-diethylammonium)hexyl-2,5-thiophene] (P3SBDEAHT) conjugated polyelectrolyte (CPE) and its interaction in water with surfactants, using absorption, photoluminescence (PL), electrical conductivity, molecular dynamics simulations (MDS) and small-angle X-ray scattering (SAXS). Different surfactants were studied to evaluate the effect of the head group and chain length on the self-assembly. PL data emphasize the importance of polymer-surfactant electrostatic interactions in the formation of complexes. Nevertheless, conductivity and MDS data have shown that nonspecific interactions also play an important role. These seem to be responsible for the spatial position of the surfactant tail in the complex and, eventually, for breaking-up P3SBDEAHT aggregates. SAXS measurements on P3SBDEAHT-zwitterionic cocamidopropyl betaine (CAPB) surfactant complexes showed a specific structural organization of the system. The CAPB surfactant promotes a structural transition from pure P3SBDEAHT 3-dimensional aggregates (radius of gyration ∼85 Å) to thick cylindrical aggregates (∼20 Å) where all CAPB molecules are associated with the polymer. For molar ratios (in terms of the polymer repeat unit) >1 the SAXS interference maximum of the complexes resembles that of pure CAPB thus suggesting ongoing phase segregation in the formation of a "pure" CAPB phase.
Iron sensitizer converts light to electrons with 92% yield

Solar energy conversion in photovoltaics or photocatalysis involves light harvesting, or sensitization, of a semiconductor or catalyst as a first step. Rare elements are frequently used for this purpose, but they are obviously not ideal for large-scale implementation. Great efforts have been made to replace the widely used ruthenium with more abundant analogues like iron, but without much success due to the very short-lived excited states of the resulting iron complexes. Here, we describe the development of an iron-nitrogen-heterocyclic-carbene sensitizer with an excited-state lifetime that is nearly a thousand-fold longer than that of traditional iron polypyridyl complexes. By the use of electron paramagnetic resonance, transient absorption spectroscopy, transient terahertz spectroscopy and quantum chemical calculations, we show that the iron complex generates photoelectrons in the conduction band of titanium dioxide with a quantum yield of 92% from the 3 MLCT (metal-to-ligand charge transfer) state. These results open up possibilities to develop solar energy-converting materials based on abundant elements.
Mathematical beauty in service of deep approach to learning

In the fall of 2014 I taught ‘02601 Introduction to Numerical Algorithms’ to a class of 86 engineering students at Technical University of Denmark. The course employed basic calculus and linear algebra to elucidate and analyse canonical algorithms of scientific computing. A major part of the course was hands-on MATLAB programming, where the algorithms were tested and applied to solve physical model-based problems. To encourage a deep approach, and discourage a surface approach to learning, I introduced into the lectures a basic but rigorous mathematical treatment of crucial theoretical points, emphasising the beauty of the underlying mathematical structure. Into this I integrated frequent and activating dialogue with the students. In section 1 I describe the course and the students in more detail. Section 2 details and justifies the pedagogical elements I introduced into the lectures; my central hypothesis is also given there. The results of the experiment are presented and discussed in section 3.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern)
Number of pages: 8
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BFI conference series: European Society for Engineering Education. Annual Conference proceedings (5010018)
Main Research Area: Mathematics, Engineering
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sefi_POSTPRINT.pdf
Links:
http://www.sefi.be/?page_id=6043
McStas and Mantid integration

McStas and Mantid are two well-established software frameworks within the neutron scattering community. McStas has been primarily used for simulating the neutron transport mechanisms in instruments, while Mantid has been primarily used for data reduction. We report here the status of our work done on the interoperability between the instrument simulation software McStas and the data reduction software Mantid. This provides a demonstration of how to successfully link together two software packages that otherwise have been developed independently, and in particular here show how this has been achieved for an instrument simulation software and a data reduction software. This paper will also provide examples of some of the expected future enhanced analysis that can be achieved from combining accurate instrument and sample simulations with software for correcting raw data. The main application of this work is to treat raw data collected at large scale neutron facilities.
Measurement of strain in InGaN/GaN nanowires and nanopyramids

The growth and optoelectronic properties of core-shell nanostructures are influenced by the strain induced by the lattice mismatch between core and shell. In contrast with planar films, nanostructures contain multiple facets that act as independent substrates for shell growth, which enables different relaxation mechanisms. In this study, X-ray diffraction data are presented that show that InGa1-N shells grown on GaN cores are strained along each of the facets independently. Reciprocal space maps reveal multiple Bragg peaks, corresponding to different parts of the shell being strained along the individual facet planes. The strained lattice constants were found from the positions of the Bragg peaks. Vegard's law and Hooke's law for an anisotropic medium were applied in order to find the composition and strain in the InGaN shells. A range of nanowire samples with different InGaN shell thicknesses were measured and it is concluded that, with an In concentration of around 30%, major strain relaxation takes place when the thickness reaches 23nm. InGaN shells of 6 and 9nm thickness remain nearly fully strained biaxially along each of the facets of the nanowires and the facets of the nanopyramids.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Glo-USA Inc., GLO AB, Lund University
Authors: Stankevic, T. (Ekstern), Mickevicius, S. (Ekstern), Nielsen, M. S. (Ekstern), Kryliouk, O. (Ekstern), Ciechonski, R. (Ekstern), Vescovi, G. (Ekstern), Bi, Z. (Ekstern), Mikkelsen, A. (Ekstern), Samuelson, L. (Ekstern), Gundlach, C. (Intern), Feidenhans'l, R. K. (Ekstern)
Number of pages: 6
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Publication date: 2015
Main Research Area: Technical/natural sciences
Microfabrication and testing of refractive hard X-ray optics

General information
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Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.6 SNIP 2.078
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.235 SNIP 2.117
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.126 SNIP 2.101
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.674 SNIP 3.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.112 SNIP 7.433
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.817 SNIP 2.339
Scopus rating (2004): SJR 1.618 SNIP 2.239
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.206 SNIP 1.618
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.31 SNIP 2.589
Scopus rating (2001): SJR 1.7 SNIP 2.059
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.009 SNIP 2.005
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.269 SNIP 1.49

Original language: English
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Microfabrication of hard x-ray lenses

This thesis deals with the development of silicon compound refractive lenses (Si-CRLs) for shaping hard x-ray beams. The CRLs are to be fabricated using state-of-the-art microfabrication techniques. The primary goal of the thesis work is to produce Si-CRLs with considerably increased structure heights and improved uniformity compared to what is currently available. To this end, established fabrication procedures are improved and the toolbox used for lens development is enriched.

The central theme of this thesis is x-ray microscopy (XRM). As a spearhead of today's materials research it provides characterization details that cannot be obtained by other means. The respective x-ray techniques largely benefit from continuously improved x-ray sources, x-ray detectors and x-ray optics. For instance, some techniques aiming for structural investigation of poly-crystalline materials directly benefit from more intense and wider line beams with narrower waists. The thesis starts with a review of alternative x-ray lenses. Si-CRLs are identified as valuable optical components that allow shaping hard x-rays efficiently and creating beam waists that are clearly in the nanometer range. They stand out by their potential for compact integration, which is cost-effective, easy to handle and stable on-axis optics. A Si-CRL comprises multiple bi-parabolic cylindrical cavities. The bi-parabolic patterns are defined lithographically and vertically transferred into the Si substrate using deep reactive ion etching (DRIE). Based on a theoretical framework for CRLs, stringent requirements on the pattern transfer are found. Most crucially, the sidewalls of the cavities must be strictly parallel. Already slight deviations from the ideal parabolic shapes result in non-uniform and broadened waists of focused x-ray beams.

Two strategies are demonstrated, which guarantee shape fidelity, while the heights of etched lenses can be increased. Both are based on defining the bi-parabolic cavities at their perimeter by trenches of uniform width, where one trench wall is comprised of sacrificial material. The two strategies differ in the way the unwanted sacrificial material inside the cavities is removed subsequent to DRIE. While the first strategy utilizes etching of the wafer using tetches of uniform width through the thickness of the wafer for releasing the sacrificial portions, the second strategy relies on thin sacrificial structures that can be oxidized and removed by selective etching. Both strategies have proven to be equally successful in achieving a substantial increase of the heights of Si-CRLs and to facilitate accurate sidewall profile control necessary for uniform x-ray focusing. A proof of manufacture in turn asks for highly precise metrology. Therefore, a mix of techniques including optical profilometry and atomic force microscopy (AFM) has been used to obtain reliable information about the detailed three-dimensional shapes of the lenses. Adequate sample preparation and measuring procedures have been developed.

Inverse replica molding in PDMS of the CRLs was established as an effective way to circumvent the limitations of AFM probes when concave surfaces need to be characterized, e.g. due to the finite lengths of AFM probes. Four different x-ray optical components have been designed, manufactured and characterized with respect to their shape. Their optical performances were tested at the European Synchrotron Radiation Facility (ESRF). Two 1D-focusing Si-CRLs suitable as condensers in hard-XRM were developed utilizing the aforementioned two different strategies. The first Si-condenser showed focusing of a 56 keV x-ray beam into a 310 μm wide line and a waist of 980 nm (FWHM) at half maximum at a focal length of 1.3 m. The second Si-condenser allowed the focusing of 17 keV x-rays into a 180 μm wide line with a waist of 430 nm (FWHM) at a focal length of 1.3 m. Both systems allow plenty of space for sample surroundings and ensure low-divergent and wide x-ray beams with narrow waists. Both results are substantial improvements to what was available at the start of this thesis work.

The challenge of making x-ray objectives in silicon by interdigitation of lenslets alternately focusing in the vertical and horizontal directions was addressed. A functioning prototype of a 2D silicon objective for use in a bright-field hard-XRM was demonstrated. The results are promising; showing acceptably low aberration and performance close to theoretical expectations. A resolution of 300 nm with 17 keV x-rays and a focal length of 300 mm was achieved. By harnessing the potential for making more compact objectives and avoiding shape defects, one could significantly improve the focusing power, transmission and numerical aperture.

Polymer injection molding was explored as a novel route for x-ray lens manufacture. A Si-CRL template was used as a master for obtaining nickel mold inserts. CRLs made of polyethylene have proven to be promising highly efficient x-ray optics. A 55 μm long line focus with a minimal waist of 770 nm (FWHM) at a focal length of 350 mm was obtained with 17 keV x-rays. A final production rate larger than 10 pieces per hour indicates the economic value of injection molded x-ray lenses, which may have applications in more readily available small laboratory x-ray instruments or medical devices.

In each case, observed non-uniformities of the shaped x-ray beams were investigated and found to be in agreement with the lens shape measurements. In iterative steps the lenses have been improved and the most recent results allow yet another whole range of improvements to be made. The fundamentals for an advanced fabrication of silicon CRLs are laid out, which will contribute to their future use in novel applications.

General information
State: Published
Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics
Microstructure and micromechanics of the heart urchin test from X-ray tomography

The microstructure of many echinoid species has long fascinated scientists because of its high porosity and outstanding mechanical properties. We have used X-ray microtomography to examine the test of Echinocardium cordatum (heart urchin), a burrowing cousin of the more commonly known sea urchins. Three-dimensional imaging demonstrates that the bulk of the test is composed of only two distinct, highly porous, fenestrated regions (stereom), in which the thickness of the struts is constant. Different degrees of porosity are achieved by varying the spacing of the struts. Drawing an analogy to vertebrate trabecular bone, where for example, human bone has a connectivity density of \( \approx 1/\text{mm}^3 \), we measure up to 150,000 strut connections per \( \text{mm}^3 \). Simulations of mechanical loading using finite element calculations indicate that the test performs at very close to the optimum expected for foams, highlighting the functional link between structure and mechanical properties.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Mütter, D. (Ekstern), Sørensen, H. O. (Ekstern), Oddershede, J. (Intern), Dalby, K. N. (Ekstern), Stipp, S. L. S. (Ekstern)
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Web of Science (2017): Indexed yes
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Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.997 SNIP 1.99 CiteScore 6.58
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.814 SNIP 2.324 CiteScore 6.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.963 SNIP 2.269 CiteScore 6.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.904 SNIP 2.125 CiteScore 5.51
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 1.808 SNIP 1.91 CiteScore 5.15
On analytic continuity of the missing Cauchy datum for Helmholtz boundary problems

We relate the domains of analytic continuation of Dirichlet and Neumann boundary data for Helmholtz problems in two or more independent variables. The domains are related à priori, locally and explicitly in terms of complex polyrectangular neighbourhoods of planar pieces of the boundary. To this end we identify and characterise a special subspace of the standard pseudodifferential operators with real-analytic symbols. The result is applicable in the estimation of the domain of analytic continuation of solutions across planar pieces of the boundary.
On the calculation of x-ray scattering signals from pairwise radial distribution functions

We derive a formulation for evaluating (time-resolved) x-ray scattering signals of solvated chemical systems, based on pairwise radial distribution functions, with the aim of this formulation to accompany molecular dynamics simulations. The
derivation is described in detail to eliminate any possible ambiguities, and the result includes a modification to the atom-type formulation which to our knowledge is previously unaccounted for. The formulation is numerically implemented and validated.

**General information**
- **State:** Published
- **Organisations:** Center for Atomic-scale Materials Design, Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, Physical and Biophysical Chemistry
- **Authors:** Dohn, A. O. (Intern), Biasin, E. (Intern), Haldrup, K. (Intern), Nielsen, M. M. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
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  - BFI (2018): BFI-level 2
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  - Web of Science (2017): Indexed Yes
  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 1.22 SJR 0.616 SNIP 0.541
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 0.791 SNIP 0.806 CiteScore 1.19
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 1.121 SNIP 0.905 CiteScore 1.5
  - BFI (2013): BFI-level 2
  - Scopus rating (2013): SJR 1.089 SNIP 0.943 CiteScore 1.62
  - ISI indexed (2013): ISI indexed yes
  - BFI (2012): BFI-level 2
  - Scopus rating (2012): SJR 1.18 SNIP 1.064 CiteScore 1.63
  - ISI indexed (2012): ISI indexed yes
  - BFI (2011): BFI-level 2
  - Scopus rating (2011): SJR 1.055 SNIP 0.931 CiteScore 1.7
  - ISI indexed (2011): ISI indexed yes
  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 1.099 SNIP 0.933
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 1.292 SNIP 1.073
  - BFI (2008): BFI-level 2
  - Scopus rating (2008): SJR 1.478 SNIP 1.075
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 1.494 SNIP 1.048
  - Scopus rating (2006): SJR 1.154 SNIP 1.012
  - Scopus rating (2005): SJR 0.955 SNIP 1.038
  - Scopus rating (2004): SJR 1.11 SNIP 1.011
  - Web of Science (2004): Indexed yes
  - Scopus rating (2003): SJR 1.244 SNIP 0.982
  - Web of Science (2003): Indexed yes
  - Scopus rating (2002): SJR 1.32 SNIP 1.084
  - Web of Science (2002): Indexed yes
On the deformation twinning of Mg AZ31B: A three-dimensional synchrotron X-ray diffraction experiment and crystal plasticity finite element model

Crystals with a hexagonal close-packed (HCP) structure are inherently anisotropic, and have a limited number of independent slip systems, which leads to strong deformation textures and reduced formability in polycrystalline products. Tension along the c-axis of the crystal ideally activates extension twinning as a deformation mode due to the lack of easy-slip systems. In this work, experiments were devised to study extension twinning in a polycrystalline Mg alloy AZ31B with a strong basal rolling texture by tensile deformation parallel to the plate normal. Three-dimensional synchrotron X-ray diffraction (3DXRD) was used to map the center-of-mass positions, volumes, orientations, elastic strains, and stress tensors of over 1400 grains in-situ up to a true strain of 1.4%. More than 700 tensile twins were observed to form in the mapped volume under deformation. The measured center-of-mass positions and grain volumes are used to construct various 3D microstructures and model them with a Crystal Plasticity Finite Element (CPFE) code. It is observed that the average grain-resolved stress did not always select the highest ranked Schmid factor twin variant. In fact, the contribution of lower ranked variants was non-negligible. The CPFE simulation indicates that there is a small variation in the stress within each grain in the elastic regime, which increases drastically upon the onset of plasticity. One of the significant outcomes of this work is the new statistical information on the interaction between twin and parent grain. It is shown that, on average, there is a small difference between the stress normal to the twin habit plane in the parent and twin, but that this is not the case for the shear acting on the habit plane.
Optimizing shape uniformity and increasing structure heights of deep reactive ion etched silicon x-ray lenses: Paper

Line-focusing compound silicon x-ray lenses with structure heights exceeding 300 μm were fabricated using deep reactive ion etching. To ensure profile uniformity over the full height, a new strategy was developed in which the perimeter of the structures was defined by trenches of constant width. The remaining sacrificial material inside the lens cavities was removed by etching through the silicon wafer. Since the wafers become fragile after through-etching, they were then adhesively bonded to a carrier wafer. Individual chips were separated using laser micro machining and the 3D shape of fabricated lenses was thoroughly characterized by a variety of means. Optical testing using synchrotron radiation with a photon energy of 56 keV yielded a 300 μm wide beam with a waist of 980 nm (full width at half maximum) at a focal length of 1.3 m. Optical aberrations are discussed in the context of the shape analysis, where a slight bowing of the lens sidewalls and an insufficiently uniform apex region are identified as resolution-limiting factors. Despite these, the proposed fabrication route proved a viable approach for producing x-ray lenses with large structure heights and provides the means to improve the resolution and capabilities of modern x-ray techniques such as x-ray microscopy and 3D x-ray diffraction.

General information
State: Published
Organisations: DTU Danchip, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
Polarized neutron powder diffraction studies of antiferromagnetic order in bulk and nanoparticle NiO

In many materials it remains a challenge to reveal the nature of magnetic correlations, including antiferromagnetism and spin disorder. Revealing the spin structure in magnetic nanoparticles is further complicated by the large incoherent neutron scattering cross section from water adsorbed at the particle surfaces and by the broadening of diffraction peaks due to the finite crystallite size. Moreover, the spin structure in magnetic nanoparticles may deviate significantly from that of the corresponding bulk material because of the low-symmetry surroundings of surface atoms and the large relative surface contribution to the magnetic anisotropy. Here we explore the potential use of polarized neutron diffraction to reveal the magnetic structure in NiO bulk and nanoparticle powders by applying the XYZ-polarization analysis method. Our investigations address in particular the spin orientation in bulk NiO and platelet-shaped NiO nanoparticles with thickness from greater than 200 nm down to 2.0 nm. The advantage of the applied method is that it is able to clearly separate the structural, the magnetic, and the spin-incoherent scattering signals for all particle sizes. For platelet-shaped particles with thickness from greater than 200 nm down to 2.2 nm we find that the spin orientation deviates about 16° from the primary (111) plane of the platelet-shaped particles. In the smallest particles (2.0 nm thick) we find the spins are oriented with a 30° average angle to the primary (111) plane of the particles. The results show that polarization analyzed neutron powder diffraction is a viable method to investigate magnetic order in powders of antiferromagnetic nanoparticles.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Institut Max von Laue-Paul Langevin, Paul Scherrer Institut
Authors: Brok, E. (Intern), Lefmann, K. (Ekstern), Deen, P. P. (Ekstern), Lebech, B. (Intern), Jacobsen, H. (Ekstern), Nilsen, G. J. (Ekstern), Keller, L. (Ekstern), Frandsen, C. (Intern)
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Polyelectrolyte Complexes of a Cationic All Conjugated Fluorene Thiophene Diblock Copolymer with Aqueous DNA

We report on the structural and colorimetric effects of interaction of aqueous \( \sim 0.06-1\% \) poly[9,9-bis(2-ethylhexyl)fluorene]-b-poly[3-6-trimethylammoniumhexyl]thiophene] bromide (PF2/6-P3TMAHT) with double-stranded DNA to form PF2/6-P3TMAHT(DNA)\( _x \) where \( x \) is the molar ratio of DNA base pairs to P3TMAHT repeat units; \( x = 0.5 \) equals the nominal charge neutralization. PF2/6-P3TMAHT forms 20–40 nm sized particles with PF2/6 core and hydrated P3TMAHT exterior. The polymer particles form loose one-dimensional chains giving micrometer long branched chains (0.19 \( \leq x \leq 0.76 \)) and subsequently randomly shaped aggregates (\( x = 1.89 \)) upon DNA addition. Compaction of the P3TMAHT block and the 20–30 nm sized core is observed for \( x = 0.38-0.76 \) and attributed to the DNA merged within P3TMAHT domain with this structure disassembling with DNA excess. Structural transformations are followed by chromic changes seen as color changes from deep red (\( x < 0.076 \)) to yellow (\( x = 0.19 \)), nearly colorless (\( x = 0.38-0.76 \)), and back to orange (\( x = 1.89 \)).
Both absorption and photoluminescence spectra display the distinct fluorene and thiophene bands and subsequent blue and red shifts when passing $x = 0.5$. Thiophene photoluminescence (PL) is significantly quenched by DNA with increasing $x$, and the changing P3TMAHT/PF2/6 band ratio allows quantitative DNA detection. Sixteen-fold dilution does not change aggregate structure, but PL is blue-shifted, indicating weakened intermolecular interactions.
Scopus rating (2006): SJR 2.369 SNIP 1.415
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.275 SNIP 1.474
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.148 SNIP 1.511
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.034 SNIP 1.47
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.118 SNIP 1.496
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.053 SNIP 1.508
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.145 SNIP 1.527
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.713 SNIP 1.8
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**Polymer injection molding of hard X-ray refractive optics**

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X-ray optics, Polymer injection molding, Deep reactive ion etching
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

**Prediction of beam hardening artefacts in computed tomography using Monte Carlo simulations**

We show how radiological images of both single and multi material samples can be simulated using the Monte Carlo simulation tool McXtrace and how these images can be used to make a three dimensional reconstruction. Good numerical agreement between the X-ray attenuation coefficient in experimental and simulated data can be obtained, which allows us to use simulated projections in the linearisation procedure for single material samples and in that way reduce beam hardening artefacts. The simulations can be used to predict beam hardening artefacts in multi material samples with complex geometry, illustrated with an example. Linearisation requires knowledge about the X-ray transmission at varying sample thickness, but in some cases homogeneous calibration phantoms are hard to manufacture, which affects the accuracy of the calibration. Using simulated data overcomes the manufacturing problems and in that way improves the calibration. (C) 2014 Elsevier B.V. All rights reserved.

**General information**
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Lund University, Technical University of Munich, University of Munich, Novo Nordisk A/S
Authors: Thomsen, M. (Ekstern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Bech, M. (Ekstern), Willner, M. (Ekstern), Pfeiffer, F. (Ekstern), Poulsen, M. (Ekstern), Lefmann, K. (Ekstern), Feidenhans'lı, R. (Ekstern)
Number of pages: 7
Pages: 314-320
Publication date: 2015
Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data

A method for the extension of the three-dimensional X-ray diffraction technique to allow the extraction of domain volume fractions in polycrystalline ferroic materials is presented. This method gives access to quantitative domain volume fractions of hundreds of independent embedded grains within a bulk sample. Such information is critical to furthering our understanding of the grainscale interactions of ferroic domains and their influence on bulk properties. The method also provides a validation tool for mesoscopic ferroic domain modelling efforts. The mathematical formulations presented here are applied to tetragonal coarse-grained Ba$_{0.88}$Ca$_{0.12}$Zr$_{0.06}$Ti$_{0.94}$O$_3$ and rhombohedral fine-grained (0.82)Bi$_{0.5}$Na$_{0.5}$TiO$_3$–(0.18)Bi$_{0.5}$K$_{0.5}$TiO$_3$ electroceramic materials. The fitted volume fraction information is used to calculate grain-scale non-$180^\circ$ ferroelectric domain switching strains. The absolute errors are found to be approximately 0.01 and 0.03% for the tetragonal and rhombohedral cases, which had maximum theoretical domain switching strains of 0.47 and 0.54%, respectively. Limitations and possible extensions of the technique are discussed.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility, The Advanced Photon Source
Authors: Oddershede, J. (Intern), Majkut, M. (Intern), Caosyd, Q. (Ekstern), Schmidt, S. (Intern), Wright, J. P. (Ekstern), Kenesei, P. (Ekstern), Daniels, J. E. (Ekstern)
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BFI (2018): BFI-level 2
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Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.572 SNIP 4.687 CiteScore 4.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.015 SNIP 5.863 CiteScore 5.32
ISI indexed (2011): ISI indexed yes
Reduction of a Ni/Spinel Catalyst for Methane Reforming

A nickel/spinel (Ni/MgAl2O4) catalyst, w(Ni) = 22 wt%, was investigated in situ during reduction with wide angle X-ray scattering (WAXS) in a laboratory setup and with anomalous small angle X-ray scattering (ASAXS) at a synchrotron source. Complementary high resolution transmission electron microscopy (HRTEM) was performed on the fresh catalyst sample. The Ni particles in the fresh catalyst sample were observed to exhibit a Ni/NiO core/shell structure. A decrease of the Ni lattice parameter is observed during the reduction in a temperature interval from 413 – 453 K, which can be related to the reduction of the NiO shell, whereby stress due to the lattice mismatch of Ni and NiO is relieved.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Individual Nanoparticle Functionality, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Experimental Surface and Nanomaterials Physics, Atomic scale modelling and materials, Norwegian University of Science and Technology, California Institute of Technology, Haldor Topsoe AS
Reversible Guest Binding in a Non-Porous FeII Coordination Polymer Host Toggles Spin Crossover

Formation of either a dimeric compound or a 1D coordination polymer of adiponitrile adducts of [Fe(bpte)]2+ (bpte = [1,2-bis(pyridin-2-ylmethyl)thio]ethane) can be controlled by the choice of counteranion. The iron(II) atoms of the bis(adiponitrile)-bridged dimeric complex [Fe2(bpte)2(μ2-(NC(CH2)4 CN))2][SbF6]4 (2) are low spin at room temperature, as are those in the polymeric adiponitrile-linked acetone solvate polymer [{[Fe(bpte)(μ2-NC(CH2)4 CN)]BPh4}2⋅Me2CO] (3⋅Me2CO). On heating 3⋅Me2CO to 80 °C, the acetone is abruptly removed with an accompanying purple to dull lavender colour change corresponding to a conversion to a high-spin compound. Cooling reveals that the desolvate 3 shows hysteretic and abrupt spin crossover (SCO) S=0↔S=2 behaviour centred at 205 K. Non-porous 3 can reversibly absorb one equivalent of acetone per iron centre to regenerate the same crystalline phase of 3⋅Me2CO concurrently reinstating a low-spin state.
Sacrificial structures for deep reactive ion etching of high-aspect ratio kinoform silicon x-ray lenses

This article describes the realization of complex high-aspect ratio silicon structures with feature dimensions from 100 μm to 100 nm by deep reactive ion etching using the Bosch process. As the exact shape of the sidewall profiles can be crucial for the proper functioning of a device, the authors investigated how sacrificial structures in the form of guarding walls and pillars may be utilized to facilitate accurate control of the etch profile. Unlike other sacrificial structuring approaches, no silicon-on-insulator substrates or multiple lithography steps are required. In addition, the safe removal of the sacrificial structures was accomplished by thermal oxidation and subsequent selective wet etching. The effects of the dimensions and relative placement of sacrificial walls and pillars on the etching result were determined through systematic experiments. The authors applied this process for exact sidewall control in the manufacture of x-ray lenses that are very sensitive to sidewall shape nonuniformities. Compound kinoform lenses for focusing hard x-rays with structure heights of 200 μm were manufactured, and the lenses were tested in terms of their focusing ability and refracting qualities using synchrotron radiation at a photon energy of 17 keV. A 180 μm long line focus with a waist of 430 nm at a focal length of 215 mm was obtained.

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BFI (2017): BFI-level 1
Search for chameleons with CAST

In this work we present a search for (solar) chameleons with the CERN Axion Solar Telescope (CAST). This novel experimental technique, in the field of dark energy research, exploits both the chameleon coupling to matter ($\beta_m$) and to photons ($\beta_\gamma$) via the Primako effect. By reducing the X-ray detection energy threshold used for axions from 1 keV to 400 eV, CAST became sensitive to the converted solar chameleon spectrum which peaks around 600 eV. Even though we have not observed any excess above background, we can provide a 95% C.L. limit for the coupling strength of chameleons to photons of $\beta_\gamma \leq 10^{11}$ for $1 < \beta_m < 10^6$.

General information

State: Published
Organisations: National Space Institute, Astrophysics, Department of Physics, Neutrons and X-rays for Materials Physics, University of Patras, Dogus University, Centre d'Etudes Nucléaires de Saclay, Russian Academy of Sciences, Max Planck Institute, University of Trieste, CERN, Universidad de Zaragoza, University of Chicago
Authors: Anastassopoulos, V. (Ekstern), Arik, M. (Ekstern), Aune, S. (Ekstern), Barth, K. (Ekstern), Belov, A. (Ekstern), Bräuninger, H. (Ekstern), Cantatore, G. (Ekstern), Carmona, J. M. (Ekstern), Cetin, S. A. (Ekstern), Christensen, F. E. (Intern), Collar, J. I. (Ekstern), Jakobsen, A. C. (Intern)
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Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 3.309 SNIP 2.265 CiteScore 4.33
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.239 SNIP 2.112 CiteScore 4.56
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.538 SNIP 1.988 CiteScore 4.82
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.707 SNIP 2.073 CiteScore 4.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 3.37 SNIP 1.677 CiteScore 3.94
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.02 SNIP 1.569 CiteScore 3.84
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 3.067 SNIP 1.433
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.862 SNIP 1.557
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.826 SNIP 1.326
Scopus rating (2007): SJR 3.003 SNIP 1.505
Scopus rating (2006): SJR 3.096 SNIP 1.376
Scopus rating (2005): SJR 2.713 SNIP 1.399
Scopus rating (2004): SJR 2.592 SNIP 1.293
Scopus rating (2003): SJR 2.931 SNIP 1.229
Scopus rating (2002): SJR 2.705 SNIP 1.214
Simulation of waviness in neutron guides

As the trend of neutron guide designs points towards longer and more complex guides, imperfections such as waviness becomes increasingly important. Simulations of guide waviness has so far been limited by a lack of reasonable waviness models. We here present a stochastic description of waviness and its implementation in the McStas simulation package. The effect of this new implementation is compared to the guide simulations without waviness and the simple, yet unphysical, waviness model implemented in McStas 1.12c and 2.0.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Hansen, U. B. (Ekstern), Bertelsen, M. (Ekstern), Bergbäck Knudsen, E. (Intern), Lefmann, K. (Ekstern)
Number of pages: 15
Pages: 45-59
Publication date: 2015
Main Research Area: Technical/natural sciences
Simulations of super-structure domain walls in two dimensional assemblies of magnetic nanoparticles

We simulate the formation of domain walls in two-dimensional assemblies of magnetic nanoparticles. Particle parameters are chosen to match recent electron holography and Lorentz microscopy studies of almost monodisperse cobalt nanoparticles assembled into regular, elongated lattices. As the particles are small enough to consist of a single magnetic domain each, their magnetic interactions can be described by a spin model in which each particle is assigned a macroscopic "superspin." Thus, the magnetic behaviour of these lattices may be compared to magnetic crystals with nanoparticle superspins taking the role of the atomic spins. The coupling is, however, different. The superspins interact only by dipolar interactions as exchange coupling between individual nanoparticles may be neglected due to interparticle spacing. We observe that it is energetically favorable to introduce domain walls oriented along the long dimension of nanoparticle assemblies rather than along the short dimension. This is unlike what is typically observed in continuous magnetic materials, where the exchange interaction introduces an energetic cost proportional to the area of the domain walls. Structural disorder, which will always be present in realistic assemblies, pins longitudinal domain walls when the external field is reversed, and makes a gradual reversal of the magnetization by migration of longitudinal domain walls possible, in agreement with previous experimental results.

General information

State: Published
Organisations: Department of Physics, Center for Electron Nanoscopy, Experimental Surface and Nanomaterials Physics, Neutrons and X-rays for Materials Physics
Authors: Jordanovic, J. (Intern), Beleggia, M. (Intern), Schiøtz, J. (Intern), Frandsen, C. (Intern)
Number of pages: 8
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Main Research Area: Technical/natural sciences

Publication Information

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Volume: 118
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ISSN (Print): 0021-8979
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.72 SJR 0.632 SNIP 0.815
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.618 SNIP 0.84 CiteScore 1.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.005 SNIP 1.18 CiteScore 2.04
Web of Science (2014): Indexed yes
Solid State Structure of Poly(9,9-dinonylfluorene)

We report on X-ray diffraction and grazing-incidence X-ray diffraction data of poly(9,9-dinonylfluorene) (PF9) in bulk, thin films and in the 1% methylcyclohexane gel. We denote the main crystalline phase as alpha phase and propose that the unit cell is monoclinic (a = 29.31 angstrom, b = 23.65 angstrom, c = 33.33 angstrom, and gamma = 84.70 degrees) in bulk and orthorhombic (a = 28.70 angstrom, b = 23.48 angstrom, and c = 33.23 angstrom) in thin films. This structure corresponds to the layered structure along the a-axis (along the elongated side chains and perpendicular to the seemingly stiff polymer chains) and to the stacking of aromatic main chain units along the b-axis. The polymer chains are aligned...
along the c-axis. Monoclinic structure agrees with the layer spacing of 14.6 angstrom, the stacking period d(040) = 5.89 angstrom and the monomer repeat distance of 8.33 angstrom. The alpha phase experiences an order-disorder transition at 170 degrees C upon heating. In the 1% methylcydohexane gel, this structural motif is maintained but with the loss of long-range order. This is interpreted as a formation of mesomorphic beta phase with an orthorhombic unit cell (a = 29.1 angstrom, b = 28.1 angstrom, and c = 16.7 angstrom). Structural analogues to other 9,9-di-n-alkyl-substituted polyfluorenes are discussed in terms of unit cell parameters and backbone geometry.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Helsinki, Bergische Universität Wuppertal
Authors: Torkkeli, M. (Ekstern), Galbrecht, F. (Ekstern), Scherf, U. (Ekstern), Knaapila, M. (Intern)
Number of pages: 7
Pages: 5244-5250
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Main Research Area: Technical/natural sciences

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  BFI (2018): BFI-level 2
  BFI (2017): BFI-level 2
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 5.76 SJR 2.557 SNIP 1.507
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 2.407 SNIP 1.638 CiteScore 5.82
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 2.534 SNIP 1.721 CiteScore 5.83
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 2.576 SNIP 1.754 CiteScore 6.09
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 2.779 SNIP 1.58 CiteScore 5.35
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 2.556 SNIP 1.593 CiteScore 5.15
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 2.51 SNIP 1.51
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 2.962 SNIP 1.533
  Web of Science (2009): Indexed yes
  BFI (2008): BFI-level 2
  Scopus rating (2008): SJR 2.819 SNIP 1.54
  Web of Science (2008): Indexed yes
  Scopus rating (2007): SJR 3.102 SNIP 1.613
  Web of Science (2007): Indexed yes
Stress heterogeneity within each individual grain of polycrystalline Zircaloy-2 is studied using a crystal plasticity finite element (CPFE) model. For this purpose, the weighted Voronoi tessellation method is used to construct 3D geometries of more than 2600 grains based on their center-of-mass positions and volumes as measured by three-dimensional X-ray diffraction (3DXRD) microscopy. The constructed microstructure is meshed with different element densities and for different numbers of grains. Then a selected group of twin and parent pairs are studied. It is shown that the measured average stress for each grain from the 3DXRD experiment is within the stress variation zone of the grain modeled in the CPFE simulation. Also, the CPFE average stress calculation for each grain is in good agreement with the measured average stress values. It is shown that upon considering the stress variations within each grain, stresses in the parent and twin are quite different if they are plotted in the global coordinate system. However, if the stress tensor is rotated into the local coordinate system of the twin habit plane, all the stress components averaged over the presented population are close, except for the shear acting on the twin plane and the transverse stress. This result is significant as it provides information needed to model such parent-twin interactions in crystal plasticity codes.
Study of 3-D stress development in parent and twin pairs of a hexagonal close-packed polycrystal: Part I - In-situ three-dimensional synchrotron X-ray diffraction measurement

High anisotropy in the elastic and plastic properties of hexagonal close-packed (hcp) structured metals not only results in drastic stress variation across grain boundaries, but also heterogeneous distributions within grains. Understanding the
mechanism of load sharing between different grains becomes more complicated when deformation twinning plays a significant role in accommodating an externally applied load. In this paper, a comprehensive study of stress development in a coarse grained strongly textured hcp polycrystal Zircaloy-2, is given using three-dimensional X-ray diffraction (3DXRD) microscopy. In-situ uniaxial straining was carried out at seven steps up to 2.7% in the macroscopic direction that favors twin formation, while center-of-mass position, crystallographic orientation, elastic strain, stress, and relative volume of each grain were measured. This information was used to reconstruct the 3D microstructure and statistically study neighborhood effects on the load sharing. The investigated volume of the sample contained 6132 grains initially, yet as a result of twin formation, 9724 grains were measured in the same volume at the last loading step. It is shown that the most favored (highest Schmid factor) twin variant contributes the most to the twin number fraction; however, if the measured local stress within each grain is used for the calculation of Schmid factor, the contribution of other variants is relatively independent of Schmid factor.
Synthesis and Characterization of FeNi/γ-Al2O3 Egg-Shell Catalyst for H2 Generation by Ammonia Decomposition

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Article number: E-19
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:

Bibliographical note
Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Synthesis and characterization of Fe–Ni/γ-Al2O3 egg-shell catalyst for H2 generation by ammonia decomposition

The Fe–Ni alloyed nanoparticles are a promising alternative to expensive ruthenium-based catalysts for a real-scale application of hydrogen generation by ammonia decomposition. In practical applications, millimeter-sized extrudates are used as catalyst supports, where the spatial distribution of the active phase should match with the type of reaction. In this work, a novel synthesis route was developed for the preparation of a Fe–Ni/γ-Al2O3 egg-shell catalyst. Egg-shell is a preferred profile considering the highly endothermic nature of ammonia decomposition reaction. The high viscosity of glycerol, used as a solvent during impregnation, prevents the fast migration of the Fe–Ni active phase solution toward the inner-core of γ-Al2O3, giving control over the large capillary pressures. The distribution profiles were analyzed at
macroscopic scale through scanning electron microscopy mapping (SEM-EDX) and optical microscopy. A three-dimensional (3-D) reconstruction of the spherical-shaped γ-Al₂O₃ was achieved using X-ray micro tomography and the Fe–Ni egg-shell spatial distribution was inspected throughout the entire volume of the support body. Transmission electron microscopy (TEM) specimen preparation using focused ion beam (FIB) milling allowed to acquire high resolution images of the Ni and Fe nanoparticles on γ-Al₂O₃, which is particularly challenging due to the crystalline nature of this support. Distinct regions of the egg-shell catalyst were analyzed through scanning TEM (STEM) and TEM. The outer-shell region showed the presence of Fe and Ni alloyed nanoparticles with a size of approximately 5nm. The egg-shell catalyst showed significant higher activity in ammonia decomposition by converting 3 times more ammonia to equilibrium conversion than either egg-white or catalyst with uniform distribution. Moreover, the egg-shell catalyst conversion only dropped 0.05% after 10h of reaction, for a space velocity of 475ml min⁻¹ g⁻¹.

**General information**

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**Organisations:** Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Neutrons and X-rays for Materials Physics  
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**Publication date:** 2015  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Applied Catalysis A: General  
**Volume:** 505  
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- BFI (2018): BFI-level 1  
- BFI (2017): BFI-level 1  
- Web of Science (2017): Indexed Yes  
- BFI (2016): BFI-level 1  
- Scopus rating (2016): CiteScore 4.26 SJR 1.178 SNIP 1.311  
- Web of Science (2016): Indexed yes  
- BFI (2015): BFI-level 1  
- Scopus rating (2015): SJR 1.203 SNIP 1.394 CiteScore 4.08  
- Web of Science (2015): Indexed yes  
- BFI (2014): BFI-level 1  
- Scopus rating (2014): SJR 1.303 SNIP 1.574 CiteScore 4.04  
- Web of Science (2014): Indexed yes  
- BFI (2013): BFI-level 1  
- Scopus rating (2013): SJR 1.426 SNIP 1.538 CiteScore 4.01  
- ISI indexed (2013): ISI indexed yes  
- Web of Science (2013): Indexed yes  
- BFI (2012): BFI-level 1  
- Scopus rating (2012): SJR 1.549 SNIP 1.615 CiteScore 3.89  
- ISI indexed (2012): ISI indexed yes  
- Web of Science (2012): Indexed yes  
- BFI (2011): BFI-level 1  
- Scopus rating (2011): SJR 1.71 SNIP 1.706 CiteScore 4.15  
- ISI indexed (2011): ISI indexed yes  
- Web of Science (2011): Indexed yes  
- BFI (2010): BFI-level 1  
- Scopus rating (2010): SJR 1.761 SNIP 1.624  
- Web of Science (2010): Indexed yes  
- BFI (2009): BFI-level 1  
- Scopus rating (2009): SJR 1.761 SNIP 1.814  
- Web of Science (2009): Indexed yes  
- BFI (2008): BFI-level 2  
- Scopus rating (2008): SJR 1.853 SNIP 1.763
Temperature dependent polarization reversal mechanism in 0.94(Bi_{1/2}Na_{1/2})TiO_3-0.06Ba(zr_{0.02}Ti_{0.98})O_3 relaxor ceramics

The temperature at which the electric field induced long-range ordered ferroelectric state undergoes transition into the short-range ordered relaxor state, $T_{F-R}$, is commonly defined by the onset of strong dispersion of the dielectric permittivity. However, this combined macroscopic property and structural investigation of the polarization reversal process in the prototypical lead-free relaxor 0.94(Bi_{1/2}Na_{1/2})TiO_3-0.06Ba(zr_{0.02}Ti_{0.98})O_3 reveals that an applied electric field can trigger depolarization and onset of relaxor-like behavior well below $T_{F-R}$. The polarization reversal process can as such be described as a combination of (1) ferroelectric domain switching and (2) a reversible phase transition between two polar ferroelectric states mediated by a non-polar relaxor state. Furthermore, the threshold fields of the second, mediated polarization reversal mechanism depend strongly on temperature. These results are concomitant with a continuous ferroelectric to relaxor transition occurring over a broad temperature range, during which mixed behavior is observed. The nature of polarization reversal can be illustrated in electric-field-temperature (E-T) diagrams showing the electric field amplitudes associated with different polarization reversal processes. Such diagrams are useful tools for identifying the best operational temperature regimes for a given composition in actuator applications.
The IAXO Helioscope

The IAXO (International Axion Experiment) is a fourth generation helioscope with a sensitivity, in terms of detectable signal counts, at least 104 better than CAST phase-I, resulting in sensitivity on gamma one order of magnitude better. To achieve this performance IAXO will count on a 8-coil toroidal magnet with 60 cm diameter bores and equipped with X-ray focusing optics into 0.20 cm² spots coupled to ultra-low background Micromegas X-ray detectors. The magnet will be on a platform that will allow solar tracking for 12 hours per day. The next short term objectives are to prepare a Technical Design Report and to construct the first prototypes of the hardware main ingredients: demonstration coil, X-ray optics and low background detector while refining the physics case and studying the feasibility studies for Dark Matter axions.

General information

State: Published
Organisations: National Space Institute, Astrophysics, Neutrons and X-rays for Materials Physics, CEA Saclay, University of South Carolina, CERN, University of Trieste, University of Zaragoza, Lawrence Livermore National Laboratory
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Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physics: Conference Series
Volume: 650
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ISSN (Print): 1742-6596
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.383
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.288 SNIP 0.344
The microscopic structure of charge density waves in underdoped YBa$_2$Cu$_3$O$_{6.54}$ revealed by X-ray diffraction

Charge density wave (CDW) order appears throughout the underdoped high-temperature cuprate superconductors, but the underlying symmetry breaking and the origin of the CDW remain unclear. We use X-ray diffraction to determine the microscopic structure of the CDWs in an archetypical cuprate YBa$_2$Cu$_3$O$_{6.54}$ at its superconducting transition temperature ∼60 K. We find that the CDWs in this material break the mirror symmetry of the CuO$_2$ bilayers. The ionic displacements in the CDWs have two components, which are perpendicular and parallel to the CuO$_2$ planes, and are out of phase with each other. The planar oxygen atoms have the largest displacements, perpendicular to the CuO$_2$ planes. Our results allow many electronic properties of the underdoped cuprates to be understood. For instance, the CDWs will lead to local variations in the electronic structure, giving an explicit explanation of density-wave states with broken symmetry observed in scanning tunnelling microscopy and soft X-ray measurements.
The Next Generation of Axion Helioscopes: The International Axion Observatory (IAXO)

The International Axion Observatory (IAXO) is a proposed 4th-generation axion helioscope with the primary physics research goal to search for solar axions via their Primakoff conversion into photons of 1 – 10 keV energies in a strong magnetic field. IAXO will achieve a sensitivity to the axion-photon coupling gay down to a few $10^{-12}$ GeV$^{-1}$ for a wide range of axion masses up to $\sim 0.25$eV. This is an improvement over the currently best (3rd generation) axion helioscope, the CERN Axion Solar Telescope (CAST), of about 5 orders of magnitude in signal strength, corresponding to a factor $\sim 20$ in the axion photon coupling. IAXO's sensitivity relies on the construction of a large superconducting 8-coil toroidal magnet of 20 m length optimized for axion research. Each of the eight 60cm diameter magnet bores is equipped with x-ray optics focusing the signal photons into $\sim 0.2$cm$^2$ spots that are imaged by very low background x-ray detectors. The magnet will be built into a structure with elevation and azimuth drives that will allow solar tracking for 12 hours each day. This contribution is a summary of our papers [1–3] and we refer to these for further details.
We have used replica molding and large-range atomic force microscopy to characterize the three-dimensional shape of high aspect ratio microstructures. Casting inverted replicas of microstructures using polydimethylsiloxane (PDMS) circumvents the inability of AFM probes to measure deep and narrow cavities. We investigated cylindrical deep reactive ion etched cavities in silicon wafers and determined the radius of curvature (ROC) of the sidewalls as a function of depth. Statistical analysis verified the reliability and reproducibility of the replication procedure. The mean ROC was determined as $(6.32 \pm 0.06)$ lm, i.e., with 1% accuracy, while the ROC linearly increases by $(0.52 \pm 0.03)$ lm from the top to the bottom of the sidewalls. Nanometer sized surface defects are also well replicated. In addition, the method allows combining multiple features from differently processed wafers into a single sample, accelerating characterization in process optimization tasks. To access the sidewall shape samples needed to be cleaved. The method was applied to study X-ray refractive optics, whose performance is crucially affected by their three-dimensional shapes.
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.602 SNIP 1.001 CiteScore 1.45
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.745 SNIP 0.983 CiteScore 1.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.818 SNIP 1.169 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.946 SNIP 1.119
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.847 SNIP 1.127
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.05 SNIP 1.077
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.065 SNIP 1.155
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.979 SNIP 1.101
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.96 SNIP 1.001
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.99 SNIP 1.117
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.814 SNIP 0.986
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.726 SNIP 0.722
Scopus rating (2001): SJR 0.552 SNIP 0.646
Scopus rating (2000): SJR 0.748 SNIP 0.573
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.654 SNIP 0.574
Original language: English
High-aspect ratio microstructures, Atomic force microscopy, Replication molding, X-ray optics
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Publication: Research - peer-review → Journal article – Annual report year: 2015

**Time and Space resolved Methods: general discussion**

**General information**

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Discussion summary from one of more discussion meetings that focus on rapidly developing areas of chemistry.

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**Tre tigerspring for materialeforskningen**

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Aarhus University, University of Copenhagen
Authors: Willendrup, P. K. (Intern), Jørgensen, M. R. V. (Ekstern), Lefmann, K. (Ekstern), Haldrup, K. (Intern)
Number of pages: 6
Pages: 8-13
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Main Research Area: Technical/natural sciences

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Original language: Danish
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Tre tigerspring for materialeforskningen
Source: FindIt
Source-ID: 2264472706
Publication: Communication › Journal article – Annual report year: 2015

**Uncertainty budget for determinations of mean isomer shift from Mössbauer spectra**

**General information**
State: Published
Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Royal Institution of Great Britain, Physikalisch-Technische Bundesanstalt
Authors: Fock, J. (Intern), Bogart, L. (Ekstern), Posth, O. (Ekstern), Hansen, M. F. (Intern), Pankhurst, Q. (Ekstern), Frandsen, C. (Intern)
Publication date: 2015
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Main Research Area: Technical/natural sciences
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Hyperfine_interaction2015_uncertaintyBudget_vs3_LKB2.pdf
Source: PublicationPreSubmission
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Publication: Research - peer-review › Poster – Annual report year: 2015

**Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses**

Ultrafast photoinduced electron transfer preceding energy equilibration still poses many experimental and conceptual challenges to the optimization of photoconversion since an atomic-scale description has so far been beyond reach. Here we combine femtosecond transient optical absorption spectroscopy with ultrafast X-ray emission spectroscopy and diffuse X-ray scattering at the SACLA facility to track the non-equilibrated electronic and structural dynamics within a bimetallic donor–acceptor complex that contains an optically dark centre. Exploiting the 100-fold increase in temporal resolution as compared with storage ring facilities, these measurements constitute the first X-ray-based visualization of a non-equilibrated intramolecular electron transfer process over large interatomic distances. Experimental and theoretical results establish that mediation through electronically excited molecular states is a key mechanistic feature. The present study demonstrates the extensive potential of femtosecond X-ray techniques as diagnostics of non-adiabatic electron transfer processes in synthetic and biological systems, and some directions for future studies, are outlined.

**General information**
3D -Ray Diffraction Microscopy

Three-dimensional X-ray diffraction (3DXRD) microscopy is a fast and non-destructive structural characterization technique aimed at the study of individual crystalline elements (grains or subgrains) within mm-sized polycrystalline specimens. It is based on two principles: the use of highly penetrating hard X-rays from a synchrotron source and the
application of “tomographic” reconstruction algorithms for the analysis of the diffraction data. In favorable cases, the position, morphology, phase, and crystallographic orientation can be derived for up to a thousand elements simultaneously. For each grain its average strain tensor may also be derived, from which the type-II stresses can be inferred. Furthermore, the dynamics of the individual elements can be monitored during typical processes such as deformation or annealing. Hence, information on the interaction between elements can be obtained directly. In this chapter we first provide an overview of the various experimental approaches for 3DXRD that have emerged. Following this, a more detailed presentation of work related to the classical 3DXRD setup is given. Some emphasis is also placed on the mathematical challenges inherent to the reconstruction of grain and orientation maps.

**General information**

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Wind Energy, Materials science and characterization, Department of Energy Conversion and Storage, University of Copenhagen, European Synchrotron Radiation Facility, Institut National des Sciences Appliquees de Lyon, European Synchrotron Research Facility
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Title of host publication: Strain and Dislocation Gradients from Diffraction : Spatially-Resolved Local Structure and Defects
Publisher: World Scientific Publishing Co Pte Ltd
Authors: Farhi, E. (Ekstern), Monzat, C. (Ekstern), Arnerin, R. (Ekstern), van Vuuren, T. (Ekstern), Castán-Guerrero, C. (Ekstern), Hennane, C. (Ekstern), Harraud, P. A. (Ekstern), Campioni, G. (Ekstern), Fuard, S. (Ekstern), Ollivier, J. (Ekstern), Willendrup, P. K. (Intern)
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Main Research Area: Technical/natural sciences

**Advanced sources and optical components for the McStas neutron scattering instrument simulation package**

We present new McStas components Virtual_mcnp_input and Virtual_tripoli4_input, Virtual_mcnp_output and Virtual_tripoli_output to be used as interface for the MCNP and Tripoli neutron transport codes. Similarly, the new Lens component can be used to describe any refracting material set-up, including lenses and prisms. A new library for McStas adds the ability to describe any geometrical arrangement as a set of polygons. This feature has been implemented in most sample scattering components such as Single_crystal, Incoherent, Isotropic_Sqw (liquids/amorphous/powder), PowderN as well as in Guide_anyshape component for reflecting or absorbing complex set-up. The PSD_Detector component models a neutron absorbing gas volume, taking into account for instance the penetration depth and the associated parallax effect, the charge cloud generated at the absorption location. This gas volume can be enclosed in a scattering material in order to model the absorption and scattering in the detector housing, prior to the actual detection. An extended model of the IN5b time-of-flight spectrometer at the Institut Laue Langevin is used to simulate vanadium and powder diffractograms, making use of the gas detector component.

**General information**

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Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

Recently, an interface between the Monte Carlo code MCNPX and the neutron ray-tracing code MCNPX was developed [1, 2]. Based on the expected neutronic performance and guide geometries relevant for the ESS, the combined MCNPX-McStas code is used to calculate dose rates along neutron beam guides. The generation and moderation of neutrons is simulated using a full scale MCNPX model of the ESS target monolith. Upon entering the neutron beam extraction region, the individual neutron states are handed to McStas via the MCNPX-McStas interface. McStas transports the neutrons through the beam guide, and by using newly developed event logging capability, the neutron state parameters corresponding to un-reflected neutrons are recorded at each scattering. This information is handed back to MCNPX where it serves as neutron source input for a second MCNPX simulation. This simulation enables calculation of dose rates in the vicinity of the guide. In addition the logging mechanism is employed to record the scatterings along the guides which is exploited to simulate the supermirror quality requirements (i.e. m-values) needed at different positions along the beam guide to transport neutrons in the same guide/source setup.

General information
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Paul Scherrer Institut
Authors: Klinkby, E. B. (Intern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Lauritzen, B. (Intern), Nonbøl, E. (Intern), Bentley, P. (Ekstern), Filges, U. (Ekstern)
Number of pages: 5
Pages: 012032
Publication date: 2014
A spherical x-ray transform and hypercube sections

We investigate the problem of sampling a unit great circle on the unit sphere $S^3$ as a support of orientation distribution functions on which acts the discrete spherical x-ray transform. The circle's partition subsets are gnomonically mapped onto lines that constitute a convex polygon inside the bounding cubes of hypercube. Thus the problem of the great circle tracing is reduced to the problem of the four-dimensional cube sectioning by the plane containing the circle and the intersection figure (the polygon) vertices finding. In this paper, a fast, non-combinatorial approach for the polygon tracing within the general multi-dimensional frame is proposed.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Institute of Computational Mathematics and Mathematical Geophysics
Authors: Kazantsev, I. G. (Ekstern), Schmidt, S. (Intern)
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Scopus rating (2015): SJR 0.589 SNIP 1.09 CiteScore 0.8
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Scopus rating (2014): SJR 0.663 SNIP 1.205 CiteScore 0.69
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.433 SNIP 1.092 CiteScore 0.74
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.42 SNIP 0.863 CiteScore 0.5
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.437 SNIP 0.994 CiteScore 0.49
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.468 SNIP 0.719
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.385 SNIP 0.827
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.346 SNIP 0.419
Scopus rating (2007): SJR 0.421 SNIP 0.361
Scopus rating (2006): SJR 0.379 SNIP 1.254
Scopus rating (2005): SJR 0.167 SNIP 0.707
Scopus rating (2004): SJR 0.246 SNIP 0.775
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A strong steric hindrance effect on ground state, excited state, and charge separated state properties of a CuI-diimine complex captured by X-ray transient absorption spectroscopy

Photophysical and structural properties of a CuI diimine complex with very strong steric hindrance, $[\text{CuI(dppS)}_2]^+$ (dppS = 2,9-diphenyl-1,10-phenanthroline disulfonic acid disodium salt), are investigated by optical and X-ray transient absorption (OTA and XTA) spectroscopy. The bulky phenylsulfonic acid groups at 2,9 positions of phenanthroline ligands force the ground state and the metal-to-ligand charge-transfer (MLCT) excited state to adopt a flattened pseudo-tetrahedral coordination geometry in which the solvent access to the copper center is completely blocked. We analyzed the MLCT state dynamics and structures as well as those of the charge separated state resulting from the interfacial electron injection from the MLCT state to TiO2 nanoparticles (NPs). The OTA results show the absence of the sub-picosecond component previously assigned as the time constant for flattening, while the two observed time constants are assigned to a relatively slow intersystem crossing (ISC) rate (≈13.8 ps) and a decay rate (100 ns) of the $[\text{CuI(dppS)}_2]^+$ MLCT state in water. These results correlate well with the XTA studies that resolved a flattened tetrahedral Cu(i) coordination geometry in the ground state. Probing the 3MLCT state structure with XTA establishes that the 3MLCT state has the same oxidation state as the copper center in $[\text{CuI(dppS)}_2]^2+$ and the Cu-N distance is reduced by 0.06 Å compared to that of the ground state, accompanied by a rotation of phenyl rings located at 2,9 positions of phenanthroline. The structural dynamics of the photoinduced charge transfer process in the $[\text{CuI(dppS)}_2]^+/\text{TiO}2$ hybrid is also investigated, which suggests a more restricted environment for the complex upon binding to TiO2 NPs. Moreover, the Cu-N bond length of the oxidized state of $[\text{CuI(dppS)}_2]^+$ after electron injection to TiO2 NPs shortens by 0.05 Å compared to that in the ground state. The interpretation of these observed structural changes associated with excited and charge separated states will be discussed. These results not only set an example for applying XTA in capturing the intermediate structure of metal complex/semiconductor NP hybrids but also provide guidance for designing efficient CuI diimine complexes with optimized structures for application in solar-to-electricity conversion. This journal is

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Argonne National Laboratory, Northwestern University, Universite de Strasbourg
Authors: Huang, J. (Ekstern), Mara, M. (Ekstern), Stickrath, A. (Ekstern), Kokhan, O. (Ekstern), Harpham, M. (Ekstern), Haldrup, K. (Intern), Shelby, M. (Ekstern), Zhang, X. (Ekstern), Ruppert, R. (Ekstern), Sauvage, J. (Ekstern), Chen, L. (Ekstern)
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
Almost 35 years since their suggestion as a good solution to the strong CP-problem, axions remain one of the few viable candidates for the Dark Matter, although still eluding detection. Most of the methods for their detection are based on their coupling to photons, one of the most sensitive ones being the helioscope technique. We report on the current status of the CERN Axion Solar Telescope and the future International Axion Observatory (IAXO). Recent results from the second part of CAST phase II, where the magnet bores were filled with $^3$He gas at variable pressure, achieving sensibilities on the axion mass up to 1.2 eV, are presented. Currently, CAST is expecting to improve its sensitivity to solar axions with rest mass below 0.02 eV/c$^2$ after the upgrade of the X-ray detectors and with the implementation of a second X-ray optic. At the same time, it is exploring other possibilities at the low energy physics frontier. On the other hand, IAXO, the fourth generation axion helioscope, aims to improve CAST’s performance in terms of axion-photon coupling by 1-1.5 orders of magnitude. The details of the project building a dedicated magnet, optics and X-ray detectors are given.
Bromosubstituted norbornadienes and their reversible photolytic transformation to quadricyclanes
Two new model systems for use within the rapidly developing ultrafast time resolved x-ray scattering techniques have been prepared. Their photoisomerisation from norbornadiene to quadricyclane was found to be a suitable reaction to follow. Simulations of scattering patterns (not included in this report) showed that if heavy atoms are included in these molecular structures, then the transformation can be followed by transient x-ray scattering techniques. Two new bromosubstituted norbornadienes were synthesised and characterised. Absorption spectroscopy showed that the norbornadienes are converted quantitatively to quadricyclanes under UV irradiation. NMR studies showed that the process was fully reversible and that the norbornadienes could be completely recovered even without addition of catalysts. Furthermore, it was shown that the formation of quadricyclane from norbornadiene was unaffected by triplet sensitizers. The two new model systems synthesised thus are strong candidates for use in time resolved x-ray scattering studies both in gas and condensed phases.

CAMEA ESS: The Continuous Angle Multi-Energy Analysis Indirect Geometry Spectrometer for the European Spallation Source
The CAMEA ESS neutron spectrometer is designed to achieve a high detection efficiency in the horizontal scattering plane, and to maximize the use of the long pulse European Spallation Source. It is an indirect geometry time-of-flight spectrometer that uses crystal analysers to determine the final energy of neutrons scattered from the sample. Unlike other indirect geometry spectrometers CAMEA will use ten concentric arcs of analysers to analyse scattered neutrons at ten different final energies, which can be increased to 30 final energies by use of prismatic analysis. In this report we will outline the CAMEA instrument concept, the large performance gain, and the potential scientific advancements that can be
made with this instrument

**General information**

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**Organisations:** Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), University of Copenhagen, Paul Scherrer Institut

**Authors:** Freeman, P. (Ekstern), Birk, J. (Ekstern), Marko, M. (Ekstern), Bertelsen, M. (Ekstern), Larsen, J. (Intern), Christensen, N. B. (Intern), Lefmann, K. (Ekstern), Jacobsen, J. (Ekstern), Niedermayer, C. (Ekstern), Juranyi, F. (Ekstern), Ronnow, H. (Ekstern)

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- Web of Science (2016): Indexed yes
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- Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32
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- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25
- ISI indexed (2013): ISI indexed no
- Web of Science (2013): Indexed yes
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- Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33
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- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43
- ISI indexed (2011): ISI indexed no
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.288 SNIP 0.344
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.253 SNIP 0.321
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.265 SNIP 0.294
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 0.257 SNIP 0.39
- Web of Science (2007): Indexed yes
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Choppers to optimise the repetition rate multiplication technique on a direct geometry neutron chopper spectrometer

In recent years the use of repetition rate multiplication (RRM) on direct geometry neutron spectrometers has been established and is the common mode of operation on a growing number of instruments. However, the chopper configurations are not ideally optimised for RRM with a resultant 100 fold flux difference across a broad wavelength band. This paper presents chopper configurations that will produce a relative constant (RC) energy resolution and a relative variable (RV) energy resolution for optimised use of RRM. The RC configuration provides an almost uniform $\Delta E/E$ for all incident wavelengths and enables an efficient use of time as the entire dynamic range is probed with equivalent statistics, ideal for single shot measurements of transient phenomena. The RV energy configuration provides an almost uniform opening time at the sample for all incident wavelengths with three orders of magnitude in time resolution probed for a single European Spallation Source (ESS) period, which is ideal to probe complex relaxational behaviour. These two chopper configurations have been simulated for the Versatile Optimal Resolution direct geometry spectrometer, VOR, that will be built at ESS.
Comment on Y. Couder and E. Fort

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Authors: Andersen, A. P. (Intern), Madsen, J. (Intern), Reichelt, C. G. (Intern), Ahl, S. R. (Intern), Lautrup, B. (Ekstern), Ellegaard, C. S. (Ekstern), Levinsen, M. (Ekstern), Bohr, T. (Intern)
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Competing charge, spin, and superconducting orders in underdoped YBa2Cu3Oy
To explore the doping dependence of the recently discovered charge-density-wave (CDW) order in YBa2Cu3Oy, we present a bulk-sensitive high-energy x-ray study for several oxygen concentrations, including strongly underdoped YBa2Cu3O6.44. Combined with previous data around the so-called 1/8 doping, we show that bulk CDW order exists at least for hole concentrations (p) in the CuO2 planes of 0.078≤p≤0.132. This implies that CDW order exists in close vicinity
to the quantum critical point for spin-density-wave (SDW) order. In contrast to the pseudogap temperature $T^*$, the onset temperature of CDW order decreases with underdoping to TCDW~90 K in YBa2Cu3O6.44. Together with a weakened order parameter this suggests a competition between CDW and SDW orders. In addition, the CDW order in YBa2Cu3O6.44 shows the same type of competition with superconductivity as a function of temperature and magnetic field as samples closer to $p=1/8$. At low $p$ the CDW incommensurability continues the previously reported linear increasing trend with underdoping. In the entire doping range the in-plane correlation length of the CDW order in $b$ axis direction depends only very weakly on the hole concentration, and appears independent of the type and correlation length of the oxygen-chain order. The onset temperature of the CDW order is remarkably close to a temperature $T^\dagger$ that marks the maximum of $1/(T_1T)$ in planar $^{63}$Cu NQR/NMR experiments, potentially indicating a response of the spin dynamics to the formation of the CDW. Our discussion of these findings includes a detailed comparison to the charge stripe order in La2-xBaxCuO4.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Brookhaven National Laboratory, University of Birmingham, University of British Columbia, Deutsches Elektronen-Synchrotron, University of Bristol, Ecole Polytechnique Federale de Lausanne (EPFL)
Authors: Hücker, M. (Ekstern), Christensen, N. B. (Intern), Holmes, A. T. (Ekstern), Blackburn, E. (Ekstern), Forgan, E. M. (Ekstern), Liang, R. (Ekstern), Bonn, D. A. (Ekstern), Hardy, W. N. (Ekstern), Gutowski, O. (Ekstern), Zimmermann, M. V. (Ekstern), Hayden, S. M. (Ekstern), Chang, J. (Ekstern)
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Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.982 SNIP 1.524
Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects

By using a newly implemented QM/MM multiscale MD method to simulate the excited state dynamics of the Ir2(dimen)42+ (dimen = 1,8-diisocyano-p-menthane) complex, we not only report on results that support the two experimentally observed coherent dynamical modes in the molecule but also reveal a third mode, not distinguishable by spectroscopic methods. We directly follow the channels of energy dissipation to the solvent and report that the main cause for coherence decay is the initial wide range of configurations in the excited state population. We observe that the solvent can actually extend the coherence lifetime by blocking channels for intramolecular vibrational energy redistribution (IVR).

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Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Department of Physics, NanoChemistry, Neutrons and X-rays for Materials Physics
Authors: Dohn, A. O. (Intern), Jónsson, E. Ö. (Intern), Kjær, K. S. (Intern), Brandt van Driel, T. (Intern), Nielsen, M. M. (Intern), Jacobsen, K. W. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
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Web of Science (2017): Indexed yes
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Direct observation of grain boundary migration during recrystallization within the bulk of a moderately deformed aluminium single crystal

A single grain growing in the bulk of a mildly deformed (30% thickness reduction through cold rolling) aluminium single crystal with an (001)<100> orientation (Cube orientation), is monitored during recrystallization with synchrotron radiation using topo-tomography. The formation and migration of planar boundary segments (facets) are analyzed using a method that determines the displacements of local boundary segments along parallel lines perpendicular to the facet plane. Facets are observed to form after a certain annealing time. They migrate at a constant rate for extended periods of time and remain planar during their migration. A change in the migration rate for one facet has been observed which is not related to changes in the experimental conditions and is most likely to be driven by the changes in grain orientation and/or the local deformation microstructure. The crystallography of the analyzed facets is not closely related to any crystallographic {111} plane of neither the growing grain nor the disappearing deformed matrix. © 2013 The Japan Institute of Metals and Materials.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Wind Energy, Materials science and characterization, Department of Mechanical Engineering, Materials and Surface Engineering, University of Manchester, Institut National des Sciences Appliquees de Lyon
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Efficient Analytical Approaches to the Optics of Compound Refractive Lenses for Use with Synchrotron X-rays

The properties of compound refractive lenses (CRLs) of biconcave parabolic lenses for focusing and imaging synchrotron X-rays have been investigated theoretically by ray transfer matrix analysis and Gaussian beam propagation. We present approximate analytical expressions, that allow fast estimation of the CRL characteristics, and build intuition into the design
of advanced CRL optics.

**General information**
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Northwestern University
Authors: Poulsen, S. O. (Ekstern), Poulsen, H. F. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.231 SNIP 1.332 CiteScore 1.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.671 SNIP 1.877 CiteScore 2.06
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.481 SNIP 1.63 CiteScore 1.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.419 SNIP 1.706 CiteScore 1.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.508 SNIP 1.703 CiteScore 1.78
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.688 SNIP 1.802
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.608 SNIP 1.53
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BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.505 SNIP 1.536
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.314 SNIP 1.544
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.397 SNIP 1.653
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.183 SNIP 1.414
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.078 SNIP 1.607
Epitaxial growth of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ films on $\text{Ce}_{0.9}\text{La}_{0.1}\text{O}_{2-y}$ buffered yttria-stabilized zirconia substrates by an all-chemical-solution route

In view of high rate fabrication of coated conductors at low-cost, YBa2Cu3O7 (YBCO) films on Ce0.9La0.1O2−y buffered yttria-stabilized zirconia substrates were deposited by means of a novel low-fluorine metal–organic solution route. A high critical current density of 3 MA cm−2 (77 K, self field) was achieved on such an all-chemical derived configuration. Structural characterization showed that the enhanced superconductivity performance of the YBCO films is mainly related to the defects induced by the interface.
Etching patterns on the micro- and nanoscale

Dry etching is widely used for realizing micro- and nanostructured devices in various materials. Here, the available dry etching techniques and their capabilities at DTU-Danchip are presented. What sets the dry etching apart from the traditional wet etching in which a chemical agent dissolved in a liquid reacts with material from the substrate is the ability to fine-tune the etch process. In wet processing the removal of material generally occurs indiscriminately of direction in the substrate - hence in all directions. This puts a strong limitation on what may be achieved in terms of designs, materials and depths. With the dry etch tools available in the cleanroom at DTU-Danchip, the etching of a great variety of materials may be tuned very precisely from a purely chemical and isotropic etch to a purely physical and anisotropic etch. The dry etching of silicon is the most flexible and well-established process that enables the users of our lab to realize devices on any scale in the sub 100 nm to the sub 1 mm range. The silicon compound refractive lenses (see left figure) for focusing hard X-rays from a synchrotron source are examples of etch processes with extreme specifications. In order to focus the X-ray beam down to a spot size of some 100 nm, the sidewalls of the cavities etched down to 300 μm into a silicon wafer must be perfectly straight and normal to the surface and have minimum roughness. The range of possible applications of the silicon etches is greatly extended if combined with electroplating and polymer injection molding. High precision patterns of, for instance microfluidic devices, are etched into silicon which is then electroplated with nickel that will serve as a stamp in the polymer injection molding tool where thousands of devices may be replicated. In addition to silicon and its derived materials such as oxides, nitrides or quartz, a lot of materials may be etched. In the ion milling tool we can etch basically any material – although at a somewhat limited depth. The ion beam that spatters off material may be tilted and devices such as blazed gratings (see right figure) may be produced.

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Publisher: Technical University of Denmark (DTU)
Main Research Area: Technical/natural sciences
Evidence for SrHo2O4 and SrDy2O4 as model J1-J2 zigzag chain materials

Neutron diffraction and inelastic spectroscopy is used to characterize the magnetic Hamiltonian of SrHo2O4 and SrDy2O4. Through a detailed computation of the crystal-field levels we find site-dependent anisotropic single-ion magnetism in both materials, and diffraction measurements show the presence of strong one-dimensional spin correlations. Our measurements indicate that competing interactions of the zigzag chain, combined with frustrated interchain interactions, play a crucial role in stabilizing spin-liquid type correlations in this series.
Excited state kinetics of anthracene-bridge-aniline intramolecular exciplexes

We report on the synthesis and characterization of fluorescent halogen substituted anthracene-bridge-aniline (ABA) supermolecules that undergo structural reorganization on photoexcitation to form transient complexes. The syntheses were achieved in high yields on a large scale and the molecular structures were confirmed by single crystal X-ray diffraction. The photophysics of the ABA supermolecules were investigated using steady state and time resolved optical spectroscopy. Despite the presence of heavy atoms the series of ABA molecules have high quantum yields of fluorescence from both a locally excited anthracene state (LE) and an excited state complex (exciplex, EP) in non-polar solvents. The kinetics of the excited state processes were established in decalin from the time-resolved emission, and was shown to be strongly influenced by an electron-transfer state (ET). For quantitative studies of the excited state dynamics, the presence of this state required the development of a numerical three-excited-state kinetic model to replace the commonly used two-excited-state model. The experimental results shows that the reaction rates are strongly influenced both by substituents and solvent, illustrating the importance of including all relevant states in the kinetic modeling. Ultimately it is established that the excited state dynamics can conveniently be followed by optical methods, and the applicability of the system as a model system in time-resolved X-ray scattering experiments is discussed.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Lund University, University of Copenhagen
Authors: Thyrhaug, E. (Ekstern), Hammershøj, P. (Ekstern), Kjær, K. S. (Intern), Sørensen, T. J. (Ekstern), Harrit, N. H. (Ekstern), Nielsen, M. M. (Intern), Bechgaard, K. (Ekstern)
Number of pages: 13
Pages: 1093-1105
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Photochemical & Photobiological Sciences
Volume: 13
Issue number: 7
ISSN (Print): 1474-905X
Ratings:
BFI (2018): BFI-level 1
Full 3D characterization of high aspect ratio microstructures

General information
State: Published
Organisations: DTU Danchip, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Danish Fundamental Metrology
Publication date: 2014
Event: Poster session presented at 40th International Conference on Micro and Nano Engineering, Lausanne, Switzerland.
Main Research Area: Technical/natural sciences
Grain centre mapping - 3DXRD measurements of average grain characteristics.

Three-Dimensional X-ray Diffraction (3DXRD) Microscopy is a generic term covering a variety of different techniques for characterising the microstructure within the bulk of polycrystalline materials. One strategy, namely grain centre mapping, enables fast measurements of the average characteristics of each grain (such as their centre-of-mass positions, volumes, phases, orientations and/or elastic strain tensor components), while the exact locations of the grain boundaries are unknown. In the present chapter, a detailed description of the setup and software for both grain centre mapping and the closely related boxscan method is given. Both validation experiments and applications for in situ studies of microstructural changes during plastic deformation and crack growth are given. Finally, an outlook with special emphasis on coupling the measured results with modelling is given.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Mechanical Engineering, Materials and Surface Engineering, European Synchrotron Research Facility
Authors: Oddershede, J. (Intern), Schmidt, S. (Intern), Lyckegaard, A. (Intern), Lauridsen, E. M. (Intern), Wright, J. P. (Ekstern), Winther, G. (Intern)
Publication date: 2014

Host publication information
Title of host publication: Strain and Dislocation Gradients from Diffraction: Spatially-Resolved Local Structure and Defects.
Publisher: World Scientific Publishing Co Pte Ltd
Editors: Barabash, R., Ice, G.
Chapter: 7
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2014

GrainSpotter: a fast and robust polycrystalline indexing algorithm

A new approach for indexing multigrain diffraction data is presented. It is based on the use of a monochromatic beam simultaneously illuminating all grains. By operating in sub-volumes of Rodrigues space, a powerful vertex-finding algorithm can be applied, with a running time that is compatible with online analysis. The resulting program, GrainSpotter, is sufficiently fast to enable online analysis during synchrotron sessions. The program applies outlier rejection schemes, leading to more robust and accurate data. By simulations it is shown that several thousand grains can be retrieved. A new method to derive partial symmetries, called pseudo-twins, is introduced. Uniquely, GrainSpotter includes an analysis of pseudo-twins, which is shown to be critical to avoid erroneous grains resulting from the indexing.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Schmidt, S. (Intern)
Pages: 276-284
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Crystallography
Volume: 47
Issue number: 1
ISSN (Print): 0021-8898
Ratings:
BFI (2018): BFI-level 2
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
High-field re-entrance of the magnetoelectric effect in LiNiPO₄ investigated in pulsed fields

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Oak Ridge National Laboratory, Helmholtz-Zentrum Berlin für Materialien und Energie, Tohoku University, Iowa State University
Number of pages: 1
Publication date: 2014
Event: Poster session presented at 4th Annual Niels Bohr International Academy Workshop-School on ESS Science, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions: highFieldPoster.pdf

Relations
Activities:
4th Annual Niels Bohr International Academy Workshop-School on ESS Science
Publication: Research - peer-review › Poster – Annual report year: 2014

High-Resolution Reciprocal Space Mapping for Characterizing Deformation Structures
With high-angular resolution three-dimensional X-ray diffraction (3DXRD), quantitative information is gained about dislocation structures in individual grains in the bulk of a macroscopic specimen by acquiring reciprocal space maps. In high-resolution 3D reciprocal space maps of tensile-deformed copper, individual, almost dislocation-free subgrains are identified from high-intensity peaks and distinguished by their unique combination of orientation and elastic strain; dislocation walls manifest themselves as a smooth cloud of lower intensity. The elastic strain shows only minor variations within each subgrain, but larger variations between different subgrains. On average, subgrains experience backward strains, whereas dislocation walls are strained in a forward direction. Based on these observations the necessary revision of the classical composite model is outlined. Additionally, subgrain dynamics is followed in situ during varying loading conditions by reciprocal space mapping: during uninterrupted tensile deformation, formation of subgrains is observed concurrently with broadening of Bragg reflections shortly after the onset of plastic deformation. When the traction is terminated, stress relaxation occurs, but no changes in number, size and orientation of the subgrains are observed. The radial profile asymmetry becomes reversed, when pre-deformed specimens are deformed in tension along a perpendicular axis.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, Roskilde Universitet, Deutsches Elektronen-Synchrotron
Pages: 322-357
Publication date: 2014

Host publication information
Title of host publication: Strain and Dislocation Gradients from Diffraction: Spatially-Resolved Local Structure and Defects
Publisher: World Scientific Publishing Co Pte Ltd
Editors: Barabash, R., Ice, G.
ISBN (Electronic): 978-1-908979-64-3
Chapter: 9
Main Research Area: Technical/natural sciences
DOIs: 10.1142/9781908979636_0009
Publication: Research - peer-review › Book chapter – Annual report year: 2015

iFit: a new data analysis framework. Applications for data reduction and optimization of neutron scattering instrument simulations with McStas
We present a new tool, iFit, which uses a single object class to hold any data set, and provides an extensive list of methods to import and export data, view, manipulate, apply mathematical operators, optimize problems and fit models to the data sets. Currently implemented using Matlab®, the toolbox is lightweight and comes with an extensive documentation based on tutorials with ready-to-run examples for each operator. Provided with the package is a set of optimization algorithms, which we have benchmarked in order to recommend the ones that provide the best success rate
for both continuous and noisy problems. These optimizers can then be used to fit models onto data objects, and optimize McStas instrument simulations. As an application, we propose a methodology to analyse neutron scattering measurements in a pure Monte Carlo optimization procedure using McStas and iFit. As opposed to the conventional data reduction and analysis procedures, this new methodology is able to intrinsically account for most of the experimental effects, and results in the sample only model, de-convolved from the instrument.

**General information**
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Institut Laue-Langevin
Authors: Farhi, E. (Ekstern), Y., D. (Ekstern), Willendrup, P. K. (Intern)
Pages: 5-18
Publication date: 2014
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Neutron Research
Volume: 17
Issue number: 1
ISSN (Print): 1023-8166
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.313 SNIP 1.257
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.259 SNIP 2.029 CiteScore 0.88
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.101 SNIP 0
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.1 SNIP 0
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.101 SNIP 0.03
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.189 SNIP 0.153
Scopus rating (2007): SJR 0.193 SNIP 0.16
Scopus rating (2006): SJR 0.231 SNIP 0.31
Scopus rating (2005): SJR 0.144 SNIP 0.076
Scopus rating (2004): SJR 0.188 SNIP 0.111
Scopus rating (2003): SJR 0.1 SNIP 0
Scopus rating (2002): SJR 0.1 SNIP 0
Scopus rating (2001): SJR 0.1 SNIP 0
Scopus rating (2000): SJR 0.1 SNIP 0.098
Scopus rating (1999): SJR 0.121 SNIP 0.027
Original language: English
DATA analysis, Monte Carlo, Neutron scattering, Numerical analysis, Optimization
DOIs:
10.3233/JNR-130001
Publication: Research - peer-review › Journal article – Annual report year: 2014

**Incorporation of Monovalent Cations in Sulfate Green Rust**
Green rust is a naturally occurring layered mixed-valent ferrous-ferric hydroxide, which can react with a range of redox-active compounds. Sulfate-bearing green rust is generally thought to have interlayers composed of sulfate and water.
Here, we provide evidence that the interlayers also contain monovalent cations, using X-ray photoelectron spectroscopy and synchrotron X-ray scattering. For material synthesized with Na\(^+\), K\(^+\), Rb\(^+\), or Cs\(^+\), interlayer thickness derived from basal plane spacings correlates with the radius of the monovalent cation. In addition, sequential washing of the materials with water showed that Na\(^+\) and K\(^+\) were structurally fixed in the interlayer, whereas Rb\(^+\) and Cs\(^+\) could be removed, resulting in a decrease in the basal layer spacing. The incorporation of cations in the interlayer opens up new possibilities for the use of sulfate green rust for exchange reactions with both anions and cations: e.g., radioactive Cs.

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Christiansen, B. C. (Ekstern), Dideriksen, K. (Ekstern), Katz, A. (Ekstern), Nedel, S. (Ekstern), Bovet, N. (Ekstern), Sørensen, H. O. (Ekstern), Frandsen, C. (Intern), Gundlach, C. (Intern), Andersson, M. P. (Ekstern), Stipp, S. L. S. (Ekstern)
Number of pages: 8
Pages: 8887-8894
Publication date: 2014
Main Research Area: Technical/natural sciences

**Publication information**

Journal: INORGANIC CHEMISTRY
Volume: 53
Issue number: 17
ISSN (Print): 0020-1669
Ratings: BFI (2018): BFI-level 2
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.98 SNIP 1.323
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.982 SNIP 1.47
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.025 SNIP 1.412
Web of Science (2008): Indexed yes
Solar axions could be converted into x-rays inside the strong magnetic field of an axion helioscope, triggering the detection of this elusive particle. Low background x-ray detectors are an essential component for the sensitivity of these searches. We report on the latest developments of the Micromegas detectors for the CERN Axion Solar Telescope (CAST), including technological pathfinder activities for the future International Axion Observatory (IAXO). The use of low background techniques and the application of discrimination algorithms based on the high granularity of the readout have led to background levels below $10^{-6}$ counts/keV/cm²/s, more than a factor 100 lower than the first generation of Micromegas detectors. The best levels achieved at the Canfranc Underground Laboratory (LSC) are as low as $10^{-7}$ counts/keV/cm²/s, showing good prospects for the application of this technology in IAXO. The current background model, based on underground and surface measurements, is presented, as well as the strategies to further reduce the background level. Finally, we will describe the R&D paths to achieve sub-keV energy thresholds, which could broaden the physics case of axion helioscopes.

**Low Background Micromegas in CAST**

Solar axions could be converted into x-rays inside the strong magnetic field of an axion helioscope, triggering the detection of this elusive particle. Low background x-ray detectors are an essential component for the sensitivity of these searches. We report on the latest developments of the Micromegas detectors for the CERN Axion Solar Telescope (CAST), including technological pathfinder activities for the future International Axion Observatory (IAXO). The use of low background techniques and the application of discrimination algorithms based on the high granularity of the readout have led to background levels below $10^{-6}$ counts/keV/cm²/s, more than a factor 100 lower than the first generation of Micromegas detectors. The best levels achieved at the Canfranc Underground Laboratory (LSC) are as low as $10^{-7}$ counts/keV/cm²/s, showing good prospects for the application of this technology in IAXO. The current background model, based on underground and surface measurements, is presented, as well as the strategies to further reduce the background level. Finally, we will describe the R&D paths to achieve sub-keV energy thresholds, which could broaden the physics case of axion helioscopes.

**General information**

State: Published
Organisations: National Space Institute, Astrophysics, Department of Physics, Neutrons and X-rays for Materials Physics, Centre d'Etudes Nucléaires de Saclay, University of Zaragoza, Universidad de Zaragoza, CERN, Lawrence Livermore National Laboratory
Number of pages: 6
Publication date: 2014

**Host publication information**
The title of the host publication: Proceedings of the 7th International Symposium on "Large TPCs for Low-Energy Rare Event Detection"
The article number: 012008

Series: Journal of Physics: Conference Series (Online)
Volume: 650
ISSN: 1742-6596
Main Research Area: Technical/natural sciences
Conference: 7th International Symposium on "Large TPCs for Low-Energy Rare Event Detection", Paris, France, 15/12/2014 - 15/12/2014
Electronic versions:
1503.05107v1_1_.pdf
Magnetic ordering in TmGa

We have determined the magnetic structure of the intermetallic compound TmGa by high-resolution neutron powder diffraction and $^{169}$Tm Mössbauer spectroscopy. This compound crystallizes in the orthorhombic (Cmcm) CrB-type structure and its magnetic structure is characterized by magnetic order of the Tm sublattice along the a-axis. The initial magnetic ordering occurs at 15(1) K and yields an incommensurate antiferromagnetic structure described by the propagation vector $k_1 = [0 \, 0.275(2) \, 0]$. At 12 K the dominant ferromagnetic ordering of the Tm sublattice along the a-axis develops in what appears to be a first-order transition. At 3 K the magnetic structure of TmGa is predominantly ferromagnetic but a weakened incommensurate component remains. The ferromagnetic Tm moment reaches $6.7(2) \ \mu_B$ at 3 K and the amplitude of the remaining incommensurate component is $2.7(4) \ \mu_B$. The $^{169}$Tm hyperfine magnetic field at 5 K is 631(1) T.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays forMaterials Physics, University of New South Wales, Bragg Institute
Authors: Cadogan, J. (Ekstern), Stewart, G. (Ekstern), Muños Pérez, S. (Ekstern), Corbas, R. (Ekstern), Hansen, B. R. (Intern), Avdeev, M. (Ekstern), Hutchison, W. (Ekstern)
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physics: Condensed Matter
Volume: 26
Issue number: 11
ISSN (Print): 0953-8984
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.89 SJR 0.881 SNIP 0.754
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.824 SNIP 0.754 CiteScore 1.65
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.217 SNIP 0.951 CiteScore 1.99
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.297 SNIP 1.022 CiteScore 2.11
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.659 SNIP 1.166 CiteScore 2.33
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.627 SNIP 1.166 CiteScore 2.31
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.654 SNIP 1.053
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Manufacture of Bi-cuprate thin films on MgO single crystal substrates by chemical solution deposition
Bi2Sr2CaCu2O8 thin films have been deposited on MgO single crystal substrates by spin-coating a solution based on 2-ethylhexanoate precursors dissolved in xylene. Pyrolysis takes place between 200°C and 450°C and is accompanied by the release of 2-ethylhexanoic acid, CO2 and H2O vapour. Highly c-axis oriented Bi2Sr2CaCu2O8 as well as Er- or Ho-doped Bi2Sr2(Ca,Ln)Cu2O8 (Ln = Er, Ho) films were obtained after heat treatment at 840°C in air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Institute of Chemical Technology, University of Turku
Authors: Grivel, J. (Intern), Bertelsen, C. V. (Intern), Andersen, N. H. (Intern), Kepa, K. (Intern), Hlásek, T. (Ekstern), Rubešová, K. (Ekstern), Huhtinen, H. (Ekstern), Patuni, P. (Ekstern)
Number of pages: 4
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Conference Series (Online)
Volume: 507
Issue number: 1
Article number: 012017
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Measurement and analysis of field-induced crystallographic texture using curved position-sensitive diffraction detectors

This paper outlines measurement and analysis methodologies created for determining the structural responses of electroceramics to an electric field. A sample stage is developed to apply electric fields to ceramic materials at elevated temperatures during neutron diffraction experiments. The tested voltages and temperatures range from -20 kV to +20 kV and room temperature to 200 A degrees C, respectively. The use of the sample environment for measuring the response of ferroelectric ceramics to an electrical stimulus is demonstrated on the instrument Wombat, a monochromatic neutron diffractometer employing a curved positive sensitive detector. Methodologies are proposed to account for the geometrical effects when vector fields are applied to textured materials with angularly dispersive detector geometries. Representative results are presented for the ferroelectric (Bi\(_{1/2}\)Na\(_{1/2}\))TiO\(_3\)-6%BaTiO\(_3\) (BNT-6BT) which show both phase transformation and ferroelectric domain texturing under the application of an electric field. This experimental and analysis approach is well suited for time-resolved measurements such as stroboscopic and in situ studies on a variety of electro-active materials.

General information
Measuring and understanding ultrafast phenomena using X-rays
Within the last decade, significant advances in X-ray sources and instrumentation as well as simultaneous developments in analysis methodology has allowed the field of fast- and ultrafast time-resolved X-ray studies of solution-state systems to truly come of age. We here describe some aspects of the physics involved as well as the experimental methodology that have facilitated this development. Building on this foundation, we discuss how the information-poor, but time-resolved (difference) scattering signals can be analyzed in a quantitative model-comparison framework to provide robust information on sub-Ångstrom structural changes taking place on femtosecond to nanosecond time scales. We illustrate this approach by a presentation of recent results from the Centre for Molecular Movies at the Technical University of Denmark.

Modeling of in-vehicle magnetic refrigeration
A high-performance magnetic refrigeration device is considered as a potential technology for in-vehicle air conditioners in electric vehicles. The high power consumption of a conventional air conditioner in an electric vehicle has considerable impacts on cruising distance. For this purpose the demands on cooling power density, temperature difference between hot and cold side, transient properties and COP, will be high. In this paper the potential to reach these demands are explored for two technologies, firstly a conventional AMR device and secondly a novel magnetocaloric device based on control of the axial thermal conductivity. © 2013 Elsevier Ltd and IIR. All rights reserved.
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.344 SNIP 1.598
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.396 SNIP 1.537 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.667 SNIP 2.117 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.461 SNIP 1.979 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.426 SNIP 1.908 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.308 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.786
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.569 SNIP 1.954
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.309 SNIP 1.737
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.891 SNIP 1.646
Scopus rating (2006): SJR 1.5 SNIP 1.629
Scopus rating (2005): SJR 1.409 SNIP 1.718
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.193 SNIP 1.933
Scopus rating (2003): SJR 1.241 SNIP 1.542
Scopus rating (2002): SJR 1.592 SNIP 1.807
Scopus rating (2001): SJR 1.775 SNIP 1.86
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.001 SNIP 1.279
Scopus rating (1999): SJR 0.824 SNIP 1.213

Original language: English

THERMODYNAMICS, ENGINEERING, HEAT-TRANSFER, Active magnetic regenerator, Thermal switch, Numerical model, Magnetic refrigeration, Régénérateur magnétique actif, Modèle numérique, Froid magnétique, Interrupteur thermique, Air conditioning, Domestic appliances, Electric vehicles, Numerical models, Thermal conductivity, Active magnetic regenerators, Cooling power density, Cruising distance, High power consumption, Potential technologies, Temperature differences, Transient property

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Source-ID: 255300110
**Modelling and computation for nanoparticle reconstruction using Electron Energy Loss Spectroscopy**

**General information**
- State: Published
- Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics, University of Bremen, Institut für Werkstofftechnik
- Authors: Karamehmedovic, M. (Intern), Kiewidt, L. (Ekstern), Wriedt, T. (Ekstern)
- Number of pages: 1
- Pages: 1182
- Publication date: 2014

**Host publication information**
- Title of host publication: Book of Abstracts, META’14
- Editors: Zouhdi, S., Zheludev, N., Teng, J. H.
- Main Research Area: Technical/natural sciences
- Conference: META’14, Singapore, Singapore, 20/05/2014 - 20/05/2014
- Electronic versions:
  - Abstract_from_book_of_abstracts_1.pdf
- Links:
  - http://metaconferences.org/ocs/index.php/META14/index/pages/view/proceedings/#.VKumSHu9Hx5
- Source: PublicationPreSubmission
- Source-ID: 103643187
- Publication: Research - peer-review › Journal article – Annual report year: 2014

**Morphology Changes of Co Catalyst Nanoparticles at the Onset of Fischer-Tropsch Synthesis**

Cobalt nanoparticles play an important role as catalysts for the Fischer-Tropsch synthesis, which is an attractive route for production of synthetic fuels. It is of particular interest to understand the varying conversion rate during the first hours after introducing synthesis gas (H-2 and CO) to the system. To this end, several in situ characterization studies have previously been done on both idealized model systems and commercially relevant catalyst nanoparticles, using bulk techniques, such as X-ray powder diffraction and X-ray absorption spectroscopy. Since catalysis takes place at the surface of the cobalt particles, it is important to develop methods to gain surface-specific structural information under realistic processing conditions. We addressed this challenge using small-angle X-ray scattering (SAXS), a technique exploiting the penetrating nature of X-rays to provide information about particle morphology during in situ experiments. Simultaneous wide-angle X-ray scattering was used for monitoring the reduction from oxide to catalytically active metal cobalt, and anomalous SAXS was used for distinguishing the cobalt particles from the other phases present. After introducing the synthesis gas, we found that the slope of the scattered intensity in the Porod region increased significantly, while the scattering invariant remained essentially constant, indicating a change in the shape or surface structure of the particles. Shape- and surface change models are discussed in light of the experimental results, leading to an improved understanding of catalytic nanoparticles.

**General information**
- State: Published
- Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Norwegian University of Science and Technology, Deutsches Elektronen-Synchrotron
- Number of pages: 9
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- Publication date: 2014
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  - BFI (2018): BFI-level 1
  - BFI (2017): BFI-level 1
New developments in the McStas neutron instrument simulation package

The McStas neutron ray-tracing software package is a versatile tool for building accurate simulators of neutron scattering instruments at reactors, short- and long-pulsed spallation sources such as the European Spallation Source. McStas is extensively used for design and optimization of instruments, virtual experiments, data analysis and user training. McStas was founded as a scientific, open-source collaborative code in 1997. This contribution presents the project at its current state and gives an overview of the main new developments in McStas 2.0 (December 2012) and McStas 2.1 (expected fall
2013), including many new components, component parameter uniformisation, partial loss of backward compatibility, updated source brilliance descriptions, developments toward new tools and user interfaces, web interfaces and a new method for estimating beam losses and background from neutron optics.

**General information**

State: Published
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Paul Scherrer Institut, University of Copenhagen, Institut Laue-Langevin
Authors: Willendrup, P. K. (Intern), Bergbäck Knudsen, E. (Intern), Klinkby, E. B. (Intern), Nielsen, T. (Ekstern), Farhi, E. (Ekstern), Filges, U. (Ekstern), Lefmann, K. (Ekstern)
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- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.383
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.24 SNIP 0.373 CiteScore 0.35
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.253 SNIP 0.344 CiteScore 0.32
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.231 SNIP 0.272 CiteScore 0.25
- ISI indexed (2013): ISI indexed no
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.28 SNIP 0.354 CiteScore 0.33
- ISI indexed (2012): ISI indexed no
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.292 SNIP 0.352 CiteScore 0.43
- ISI indexed (2011): ISI indexed no
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.288 SNIP 0.344
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.253 SNIP 0.321
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.265 SNIP 0.294
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 0.257 SNIP 0.39
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 0.267 SNIP 0.284
- Web of Science (2006): Indexed yes
Original language: English
Electronic versions:
- New_developments_in_the_McStas.pdf
New developments in the McStas neutron instrument simulation package

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Nuclear Technologies, Radiation Physics, ESS Data Management & Software Center, Institut Laue-Langevin, Niels Bohr Institute, Paul Scherrer Institut
Authors: Willendrup, P. K. (Intern), Bergbäck Knudsen, E. (Intern), Klinkby, E. B. (Intern), R. Nielsen, T. (Ekstern), Farhi, E. (Ekstern), Filges, U. (Ekstern), Lefmann, K. (Ekstern)
Number of pages: 24
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Publication: Research › Sound/Visual production (digital) – Annual report year: 2015

Novel applications of the x-ray tracing software package McXtrace

We will present examples of applying the X-ray tracing software package McXtrace to different kinds of X-ray scattering experiments. In particular we will be focusing on time-resolved type experiments. Simulations of full scale experiments are particularly useful for this kind, especially when they are performed at an FEL-facility. Beamtime here is extremely scarce and the delay between experiment and publication is notoriously long. A major cause for the delay is the general complexity of the experiments performed. A complexity which arises from the pulsed state of the source. As an example, consider a pump-and-probe type experiment. In order to get the wanted signal from the sample the X-ray pulse from the FEL source needs to overlap in space and time with the pumping pulse inside the sample. This is made more difficult by several effects: The sample response may be dependent of the polarisation of the pumping and/or probing pulse. There may be significant time-jitter in the pulse arrival times. The composition of the sample may vary depending on local sample geometry and be modified by the probing pulse. Many of the samples considered are in a liquid state and thus have a variable geometry. ...to name some of the issues encountered. Generally more than one or all of these effects are present at once. Simulations can in these cases be used to identify distinct footprints of such distortions and thus give the experimenter a means of deconvoluting them from the signal. We will present a study of this kind along with the newest developments of the McXtrace software package.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, St. Olaf College
Authors: Bergbäck Knudsen, E. (Intern), Nielsen, M. M. (Intern), Haldrup, K. (Intern), Topel, E. (Ekstern), Schmidt, S. (Intern)
Number of pages: 7
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Publication date: 2014

Host publication information
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Series: Proceedings of SPIE, the International Society for Optical Engineering
Volume: 9209
ISSN: 1605-7422
Main Research Area: Technical/natural sciences
Performance of a beam-multiplexing diamond crystal monochromator at the Linac Coherent Light Source

A double-crystal diamond monochromator was recently implemented at the Linac Coherent Light Source. It enables splitting pulses generated by the free electron laser in the hard x-ray regime and thus allows the simultaneous operations of two instruments. Both monochromator crystals are High-Pressure High-Temperature grown type-IIa diamond crystal plates with the (111) orientation. The first crystal has a thickness of ~100 μm to allow high reflectivity within the Bragg bandwidth and good transmission for the other wavelengths for downstream use. The second crystal is about 300 μm thick and makes the exit beam of the monochromator parallel to the incoming beam with an offset of 600 mm. Here we present details on the monochromator design and its performance. © 2014 AIP Publishing LLC.
Preparation and Characterization of Mg1-xB2 Bulk Samples and Cu/Nb Sheathed Wires with Low Grade Amorphous Boron Powder

MgB2 bulk and wire samples were prepared using cheap, low grade amorphous boron powders. Based on chemical analysis performed on the starting reagents, three nominal stoichiometries were studied. It was found that the structural and superconducting properties of the bulk samples were not affected by the composition, but that residual Mg was left in the wires for the nominal MgB2 composition. In contrast, slightly Mg-deficient compositions were free from residual Mg and exhibited higher critical current densities. The MgB2 phase formation kinetics was not influenced by the variations in the nominal powder composition.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Institute of Chemical Technology, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Alexiou, A. (Intern), Rubesova, K. (Ekstern), Tang, X. (Intern), Andersen, N. H. (Intern), von Zimmermann, M. (Ekstern), Watenphul, A. (Ekstern)
PHYSICS,, CRITICAL-CURRENT DENSITY, SUPERCONDUCTING PROPERTIES, STARTING COMPOSITION, PRECURSOR POWDER, MGB2 WIRES, FIELD, STOICHIOMETRY, MAGNETIZATION, TAPES, PHASE, MgB2, Stoichiometry, Wires, Synchrotron, Critical current, Boron, Critical currents, Synchrotrons, Amorphous boron powder, Bulk samples, Low grade, Phase formations, Powder composition, Structural and superconducting properties, Wire, BORON, HASH(0x39fce50)
Prismatic analyzer concept for neutron spectrometers

Developments in modern neutron spectroscopy have led to typical sample sizes decreasing from few cm to several mm in diameter samples. We demonstrate how small samples together with the right choice of analyser and detector components makes distance collimation an important concept in crystal analyser spectrometers. We further show that this opens new possibilities where neutrons with different energies are reflected by the same analyser but counted in different detectors, thus improving both energy resolution and total count rate compared to conventional spectrometers. The technique can readily be combined with advanced focusing geometries and with multiplexing instrument designs. We present a combination of simulations and data showing three different energies simultaneously reflected from one analyser. Experiments were performed on a cold triple axis instrument and on a prototype inverse geometry Time-of-flight spectrometer installed at PSI, Switzerland, and shows excellent agreement with the predictions. Typical improvements will be 2.0 times finer resolution and a factor of 1.9 in flux gain compared to a focusing Rowland geometry, or of 3.3 times finer resolution and a factor of 2.4 in flux gain compared to a single flat analyser slab.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Paul Scherrer Institut, Ecole Polytechnique Federale de Lausanne (EPFL)
Authors: Birk, J. O. (Ekstern), Marko, M. (Ekstern), Freeman, P. (Ekstern), Jacobsen, J. (Ekstern), Hansen, R. L. (Ekstern), Niedermayer, C. (Ekstern), Christensen, N. B. (Intern), Måsson, M. (Ekstern), Rønnow, H. M. (Ekstern), Lefmann, K. (Ekstern)
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  Web of Science (2017): Indexed yes
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  Scopus rating (2016): CiteScore 1.2 SJR 0.585 SNIP 0.855
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 0.562 SNIP 0.824 CiteScore 1.11
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 0.922 SNIP 1.211 CiteScore 1.45
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 0.898 SNIP 1.117 CiteScore 1.28
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  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): SJR 1.012 SNIP 1.267 CiteScore 1.45
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  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 1
  Scopus rating (2011): SJR 0.861 SNIP 1.105 CiteScore 1.43
  ISI indexed (2011): ISI indexed yes
Quantum and thermal ionic motion, oxygen isotope effect, and superexchange distribution in La$_2$CuO$_4$

We study the zero-point and thermal ionic motion in La$_2$CuO$_4$ by means of high-resolution neutron-diffraction experiments. Our results demonstrate anisotropic motion of O and, to a lesser extent, Cu ions, both consistent with the structure of coupled CuO$_6$ octahedra, and quantify the relative effects of zero-point and thermal contributions to ionic motion. By substitution of O-18, we find that the oxygen isotope effect on the lattice dimensions is small and negative (~0.01%), while the isotope effect on the ionic displacement parameters is significant (~6 to 50%). We use our results as input for theoretical estimates of the distribution of magnetic interaction parameters, J, in an effective one-band model for the cuprate plane. We find that ionic motion causes only small (~1%) effects on the average value $<J>$, which vary with temperature and O isotope, but results in dramatic (10-20%) fluctuations in J values that are subject to significant (8-12%) isotope effects. We demonstrate that this motional broadening of J can have substantial effects on certain electronic and magnetic properties in cuprates.
Refractive and diffractive neutron optics with reduced chromatic aberration

Thermal neutron beams are an indispensable tool in physics research. The spatial and the temporal resolution attainable in experiments are dependent on the flux and collimation of the neutron beam which remain relatively poor, even for modern neutron sources. These difficulties may be mitigated by the use of optics for focusing and imaging. Refractive and diffractive optical elements, e.g. compound refractive lenses and Fresnel zone plates, are attractive due to their low cost, and simple alignment. These optical elements, however, suffer from chromatic aberration, which limit their effectiveness to highly monochromatic beams. This paper presents two novel concepts for focusing and imaging non-monochromatic thermal neutron beams with well-known optical elements: (1) a fast mechanical transfocator based on a compound refractive lens, which actively varies the number of individual lenses in the beam path to focus and image a time-of-flight beam, and (2) a passive optical element consisting of a compound refractive lens, and a Fresnel zone plate, which may focus and image both continuous and pulsed neutron beams.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Northwestern University
Authors: Poulsen, S. O. (Ekstern), Poulsen, H. F. (Intern), Bentley, P. (Ekstern)
Pages: 415–420
Publication date: 2014
Main Research Area: Technical/natural sciences

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Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.915 SNIP 1.334 CiteScore 1.21
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.852 SNIP 1.303 CiteScore 1.24
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.944 SNIP 1.398 CiteScore 1.48
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.806 SNIP 1.071 CiteScore 1.19
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.918 SNIP 1.424 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Rotated stripe order and its competition with superconductivity in La$_{1.88}$Sr$_{0.12}$CuO$_4$

We report the observation of a bulk charge modulation in La$_{1.88}$Sr$_{0.12}$CuO$_4$ (LSCO) with a characteristic in-plane wave vector of $(0.236, \pm \delta)$, with $\delta=0.011$ r.l.u. The transverse shift of the ordering wave vector indicates the presence of rotated charge-stripe ordering, demonstrating that the charge ordering is not pinned to the Cu-O bond direction. On cooling through the superconducting transition, we find an abrupt change in the growth of the charge correlations and a suppression of the charge order parameter indicating competition between the two orderings. Orthorhombic LSCO thus helps bridge the apparent disparities between the behavior previously observed in the tetragonal “214” cuprates and the orthorhombic yttrium and bismuth-based cuprates and thus lends strong support to the idea that there is a common motif to charge order in all cuprate families.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Brookhaven National Laboratory, Argonne National Laboratory, Hokkaido University, Muroran Institute of Technology
Authors: Thampy, V. (Ekstern), Dean, M. P. M. (Ekstern), Christensen, N. B. (Intern), Steinke, L. (Ekstern), Islam, Z. (Ekstern), Oda, M. (Ekstern), Ido, M. (Ekstern), Momono, N. (Ekstern), Wilkins, S. B. (Ekstern), Hill, J. P. (Ekstern)
Number of pages: 5
Pages: 100510
Publication date: 2014
Main Research Area: Technical/natural sciences

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Simulation and experimental validation of advanced neutron moderators

General information
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Schönfeldt, T. (Intern), Willendrup, P. K. (Intern), Lauritzen, B. (Intern), Nonbøl, E. (Intern), Klinkby, E. B. (Intern)
Number of pages: 21
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Simulations of chopper jitter at the LET neutron spectrometer at the ISIS TS2
The effect of uncertainty in chopper phasing (jitter) has been investigated for the high-resolution time-of-flight spectrometer LET at the ISIS second target station. The investigation is carried out using virtual experiments, with the neutron simulation package McStas, where the chopper jitter is found to cause a Lorentzian tail in the resolution function. We find that jitter even up to the unrealistically high value of 2 μs can be tolerated without any noticeable degradation of resolution or incident intensity. The results are supported by simple analytical estimates and are believed to be general for chopper spectrometers.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Lund University, Rutherford Appleton Laboratory
Authors: Klenø, K. H. (Ekstern), Lefmann, K. (Ekstern), Willendrup, P. K. (Intern), Christiansen, P. (Ekstern), Bewley, R. (Ekstern)
Number of pages: 9
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Main Research Area: Technical/natural sciences

Publications information
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BFI (2016): BFI-level 1
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Scopus rating (2015): SJR 0.259 SNIP 2.029 CiteScore 0.88
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
Singular value decomposition as a tool for background corrections in time-resolved XFEL scattering data

The development of new X-ray light sources, XFELs, with unprecedented time and brilliance characteristics has led to the availability of very large datasets with high time resolution and superior signal strength. The chaotic nature of the emission processes in such sources as well as entirely novel detector demands has also led to significant challenges in terms of data analysis. This paper describes a heuristic approach to datasets where spurious background contributions of a magnitude similar to (or larger than) the signal of interest prevents conventional analysis approaches. The method relies on singular-value decomposition of no-signal subsets of acquired datasets in combination with model inputs and appears generally applicable to time-resolved X-ray diffuse scattering experiments.
Small and smart magnet design

Society faces an accumulated need to find ways to produce super strong magnets that can fulfill the growing demands for green technology products such as compact and efficient generators and motors. Next-generation magnets could very likely be composite materials built bottom-up from nanoparticles. However, combining the nanoparticles into a compact magnetic material where all magnetic moments are aligned is an engineering challenge. We investigate - with nanoparticle-resolution - principles of assembly processes and particle arrangements that can generate optimal magnetic order in new materials (see e.g. Fig. 1). These studies are enabled by advanced transmission electron microscopy, magnetic modelling and new synthesis protocols. Examples of magnetic ordering and self-organization will be given.

General information

State: Published

Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, DTU Danchip, Center for Atomic-scale Materials Design, Experimental Surface and Nanomaterials Physics

Solvation dynamics monitored by combined X-ray spectroscopies and scattering: photoinduced spin transition in aqueous [Fe(bpy)3]2+

We have studied the photoinduced low spin (LS) to high spin (HS) conversion of aqueous Fe(bpy)3 with pulse-limited time resolution. In a combined setup permitting simultaneous X-ray diffuse scattering (XDS) and spectroscopic measurements at a MHz repetition rate we have unraveled the interplay between intramolecular dynamics and the intermolecular caging solvent response with 100 ps time resolution. On this time scale the ultrafast spin transition including intramolecular geometric structure changes as well as the concomitant bulk solvent heating process due to energy dissipation from the excited HS molecule are long completed. The heating is nevertheless observed to further increase due to the excess energy between HS and LS states released on a subnanosecond time scale. The analysis of the spectroscopic data allows precise determination of the excited population which efficiently reduces the number of free parameters in the XDS analysis, and both combined permit extraction of information about the structural dynamics of the first solvation shell.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European XFEL, Lund University, Argonne National Laboratory, Hungarian Academy of Sciences
Authors: Bressler, C. (Ekstern), Gawelda, W. (Ekstern), Galler, A. (Ekstern), Nielsen, M. M. (Intern), Sundström, V. (Ekstern), Doumy, G. (Ekstern), March, A. (Ekstern), Southworth, S. (Ekstern), Young, L. (Ekstern), Vanko, G. (Ekstern)
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.051 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.7 SNIP 1.278 CiteScore 3.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.618 SNIP 1.12 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 0.948 CiteScore 3.24
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.893 SNIP 1.239 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Sparse data structures in 3DXRD

In 3D X-ray diffraction tomography (3DXRD) of polycrystals, the spatial and the orientational distribution of crystal grains are numerically reconstructed from the observed diffraction spots and rings. The high dimensionality of the solution space poses a significant computational challenge. In this talk I will present a sparsity-promoting mathematical framework for the 3DXRD and show supporting numerical results.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern)
Publication date: 2014
Main Research Area: Technical/natural sciences
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Talk_titles_and_abstracts.pdf
Links:
http://www2.compute.dtu.dk/~jakj/sparsetomodays/abstracts.html
Source: PublicationPreSubmission
Source-ID: 103643233
Publication: Research › Conference abstract for conference – Annual report year: 2014

The benefit of the European User Community from transnational access to national radiation facilities

Transnational access (TNA) to national radiation sources is presently provided via programmes of the European Commission by BIOSTRUCT-X and CALIPSO with a major benefit for scientists from European countries. Entirely based on scientific merit, TNA allows all European scientists to realise synchrotron radiation experiments for addressing the Societal Challenges promoted in HORIZON2020. In addition, by TNA all European users directly take part in the development of the research infrastructure of facilities. The mutual interconnection of users and facilities is a strong prerequisite for future development of the research infrastructure of photon science. Taking into account the present programme structure of HORIZON2020, the European Synchrotron User Organization (ESUO) sees considerable dangers for the continuation of this successful collaboration in the future.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Université Lille Nord de France, Universidade Nova de Lisboa, Rudjer Boskovic Institute, Radboud University Nijmegen, Paul Scherrer Institut, University
The crystal structure of paramagnetic copper(ii) oxalate (Cu$_2$O$_4$): formation and thermal decomposition of randomly stacked anisotropic nano-sized crystallites

Synthetic copper(ii) oxalate, CuC$_2$O$_4$, was obtained in a precipitation reaction between a copper(ii) solution and an aqueous solution of oxalic acid. The product was identified from its conventional X-ray powder patterns which match that of the copper mineral Moolooite reported to have the composition CuC$_2$O$_4$·0.44H$_2$O. Time resolved in situ investigations of the thermal decomposition of copper(ii) oxalate using synchrotron X-ray powder diffraction showed that in air the compound converts to Cu$_2$O at 215 °C and oxidizes to CuO at 345 °C. Thermo gravimetric analysis performed in an inert Ar-gas reveals that the material contains no crystal water and reduces to pure Cu at 295 °C. Magnetic susceptibility measurements in the temperature range from 2 K to 300 K show intriguing paramagnetic behaviour with no sign of magnetic order down to 2 K. A crystal structure investigation is made based on powder diffraction data using one neutron diffraction pattern obtained at 5 K ($\lambda = 1.5949(1)$ Å) combined with one conventional and two synchrotron X-ray diffraction patterns obtained at ambient temperature using $\lambda = 1.54056$, 1.0981 and $\lambda = 0.50483(1)$ Å, respectively. Based on the X-ray synchrotron data the resulting crystal structure is described in the monoclinic space group $P2_1/c$ (#14) in the $P12_1/n1$ setting with unit cell parameters a = 5.9598(1) Å, b = 5.6089(1) Å, c = 5.1138 (1) Å, $\beta = 115.320(1)^\circ$. The composition is CuC$_2$O$_4$ with atomic coordinates determined by FullProf refinement of the neutron diffraction data. The crystal structure consists of a random stacking of CuC$_2$O$_4$ micro-crystallites where half the Cu-atoms are placed at (2a) and the other half at (2b) positions with the corresponding oxalate molecules centred around the corresponding (2b) and (2a) site positions, respectively. The diffraction patterns obtained for both kinds of radiation show considerable broadening of several Bragg peaks caused by highly anisotropic microstructural size and strain effects. In contrast to the water reported to be present in Moolooite, neither thermogravimetric nor the in situ thermal decomposition investigations and crystal structure analysis of the neutron diffraction data revealed any trace of water. An appendix contains details about the profile parameters for the diffractometers used at the European Synchrotron Radiation Facility and the Institute Max von Laue-Paul Langevin.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Crystal Chemistry
Authors: Christensen, A. N. (Ekstern), Lebech, B. (Intern), Andersen, N. H. (Intern), Grivel, J. (Intern)
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  Web of Science (2017): Indexed Yes
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  Scopus rating (2016): CiteScore 3.85 SJR 1.243 SNIP 0.931
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
  Web of Science (2014): Indexed yes
The upgraded cold neutron three-axis spectrometer FLEXX at BER II at HZB

Larmor labeling is seen as one of the key ingredients in the development of novel neutron instrumentation. FLEXX puts special emphasis on exploiting the neutron resonance spin echo (NRSE) technique for high-resolution spectroscopy on dispersive quasi-particle excitations. This enables unique measurements in single crystal spectroscopy over large portions of the Brillouin zone. To keep the experimental opportunities at BER II at the forefront the NRSE option available at FLEXX was upgraded along with the change of the primary spectrometer [11]. In user service upgraded V2/FLEXX provides new capabilities for quantum magnetism, heavy-fermion systems and unconventional superconductivity. For example inelastic experiments in magnetic fields up to 17 T are now proven to be feasible. Energy research with inelastic neutron instruments will be strengthened through inhouse research, thereby fostering collaborations with external partners. The research themes at the new FLEXX spectrometer in future will be centered on transport properties in
Three-Dimensional Characterization of X-ray Refractive Optics

Three-Dimensional Characterization of X-ray Refractive Optics

General information
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Organisations: DTU Danchip, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Danish Fundamental Metrology, European Synchrotron Radiation Facility
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X-ray optics, Optical profilometry, Atomic force microscopy, Replica molding
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Source: PublicationPreSubmission
Source-ID: 104505308
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Tracking excited-state charge and spin dynamics in iron coordination complexes
Crucial to many light-driven processes in transition metal complexes is the absorption and dissipation of energy by 3d electrons(1-4). But a detailed understanding of such non-equilibrium excited-state dynamics and their interplay with structural changes is challenging: a multitude of excited states and possible transitions result in phenomena too complex.
to unravel when faced with the indirect sensitivity of optical spectroscopy to spin dynamics(5) and the flux limitations of ultrafast X-ray sources(6,7). Such a situation exists for archetypal poly-pyridyl iron complexes, such as [Fe(2,2'-bipyridine)(3)](2+), where the excited-state charge and spin dynamics involved in the transition from a low-to a high-spin state (spin crossover) have long been a source of interest and controversy(6-15). Here we demonstrate that femtosecond resolution X-ray fluorescence spectroscopy, with its sensitivity to spin state, can elucidate the spin crossover dynamics of [Fe(2,2'-bipyridine)(3)](2+) on photoinduced metal-to-ligand charge transfer excitation. We are able to track the charge and spin dynamics, and establish the critical role of intermediate spin states in the crossover mechanism. We anticipate that these capabilities will make our method a valuable tool for mapping in unprecedented detail the fundamental electronic excited-state dynamics that underpin many useful light-triggered molecular phenomena involving 3d transition metal complexes.
We describe a method to measure ultrafast protein structural changes using time-resolved wide-angle X-ray scattering at an X-ray free-electron laser. We demonstrated this approach using multiphoton excitation of the Blastochloris viridis photosynthetic reaction center, observing an ultrafast global conformational change that arises within picoseconds and precedes the propagation of heat through the protein. This provides direct structural evidence for a ‘protein quake’: the hypothesis that proteins rapidly dissipate energy through quake-like structural motions.
A high-mobility two-dimensional electron gas at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃

The discovery of two-dimensional electron gases at the heterointerface between two insulating perovskite-type oxides, such as LaAlO₃ and SrTiO₃, provides opportunities for a new generation of all-oxide electronic devices. Key challenges remain for achieving interfacial electron mobilities much beyond the current value of approximately 1,000 cm²V⁻¹ s⁻¹ (at low temperatures). Here we create a new type of two-dimensional electron gas at the heterointerface between SrTiO₃ and a spinel γ-Al₂O₃ epitaxial film with compatible oxygen ions sublattices. Electron mobilities more than one order of magnitude higher than those of hitherto-investigated perovskite-type interfaces are obtained. The spinel/perovskite twodimensional electron gas, where the two-dimensional conduction character is revealed by quantum magnetoresistance oscillations, is found to result from interface-stabilized oxygen vacancies confined within a layer of 0.9 nm in proximity to the interface. Our findings pave the way for studies of mesoscopic physics with complex oxides and design of high-mobility all-oxide electronic devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, Imaging and Structural Analysis, Secretariat, IT, Management, Chinese Academy of Sciences, Leibniz Institute for Solid State and Materials Research Dresden, University of Copenhagen
Number of pages: 6
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Communications
A high-mobility two-dimensional electron gas at the spinel/perovskite interface of \(\gamma\)-Al\(_2\)O\(_3\)/SrTiO\(_3\)

The realization of high-mobility 2DEGs in epitaxially grown heterostructures made of traditional semiconductors is at the heart of present electronics, which has led to a wealth of new physical phenomena as well as new electronic and photonic devices over the past few decades. 2DEGs at the interface between insulating complex oxides not only provide a wealth of opportunities to study mesoscopic physics with strongly correlated electrons confined in nanostructures, but also show promise for multifunctional all-oxide devices with probably even richer behavior than those we experienced in semiconductor devices.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, Imaging and Structural Analysis
Number of pages: 1
Publication date: 2013
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Main Research Area: Technical/natural sciences
Electronic versions:
High_mobility_2DEGs.pdf
Source: dtu
Source-ID: u::8988
Publication: Research - peer-review › Poster – Annual report year: 2013

Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

Recently, an interface between the Monte Carlo code MCNPX and the neutron ray-tracing code MCNPX was developed[1]. Based on the expected neutronic performance and guide geometries relevant for the ESS, the combined MCNPX-McStas code is used to calculate dose rates along neutron beam guides. The generation and moderation of neutrons is simulated using a full scale MCNPX model of the ESS target monolith. Upon entering the beam extraction
region, the individual neutron states are handed to McStas via the MCNPX-McStas interface. McStas transports the neutrons through the beam guide and by using newly developed event logging capability, the neutron state parameters corresponding to un-reflected neutrons are recorded at each scattering. This information is handed back to MCNPX where it serves as neutron source input for a second MCNPX simulation. This simulation enables calculation of dose rates in the vicinity of the guide. In addition the logging mechanism is employed to record the scatterings along the guides which is exploited to simulate the supermirror quality requirements (i.e. m-values) needed at different positions along the beam guide to transport neutrons in the same guide/source setup.

**General information**
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Paul Scherrer Institut
Authors: Klinkby, E. B. (Intern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Lauritzen, B. (Intern), Nonbøl, E. (Intern), Bentley, P. (Ekstern), Filges, U. (Ekstern)
Number of pages: 6
Publication date: 2013

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Main Research Area: Technical/natural sciences
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Electronic versions: Application_of_the_MCNPX.pdf
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

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**A Two-Dimensional Electron Gas at the Spinel/Perovskite Interface of γ-Al₂O₃/SrTiO₃ with Carrier Mobility Exceeding 100,000 cm²V⁻¹s⁻¹**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy, Imaging and Structural Analysis, Chinese Academy of Sciences, Leibniz Institute for Solid State and Materials Research Dresden, University of Copenhagen
Authors: Chen, Y. (Intern), Bovet, N. (Ekstern), Trier, F. (Intern), Christensen, D. V. (Intern), Qu, F. (Ekstern), Andersen, N. H. (Intern), Kasama, T. (Intern), Zhang, W. (Intern), Giraud, R. (Ekstern), Dufouleur, J. (Ekstern), Jespersen, T. S. (Ekstern), Sun, J. (Ekstern), Smith, A. (Intern), Nygård, J. (Ekstern), Büchner, B. (Ekstern), Shen, B. (Ekstern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2013
Event: Abstract from 20th Workshop on Oxide Electronics (WOE20), Singapore, Singapore.
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Source: dtu
Source-ID: u::8989
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

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**Effect of CuF₂ on the Synthesis and Superconducting Properties of (Bi,Pb)₂Sr₂Ca₂Cu₃O₁₀ Bulk Ceramic Samples**
Bulk polycrystalline samples with Bi₁.7₂Pb₀.3₄Sr₁.87Ca₁.9₁Cu₃.1₃O₉.₈₃−ₓFₓ (0.00≤ₓ≤0.5₁) were prepared by a solid-state route using CuF₂ as a fluorine source. CuF₂ was introduced in the precursor powders either by direct mixing with the other starting reagents or by addition to precalcined precursors. In both cases, CuF₂ resulted in a clear lowering of the reaction temperature. The superconducting and secondary phase grains are larger in the CuF₂ doped samples but the critical transition temperature and the lattice parameters of the high Tc phase are not affected. EDS analysis shows that the fluorine is concentrated in SrF₂ particles.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Grivel, J. (Intern), Andersen, N. H. (Intern)
Pages: 3049-3056
Publication date: 2013
Main Research Area: Technical/natural sciences

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E-learning neutron scattering

E-learning offers a wide range of possibilities for evaluation and directly measuring how the students use the material and learn. This is made possible since all clicks and replies in quizzes etc. are stored in a database on which web analytics tools can be applied.
Femtosecond structural dynamics of spin-crossover compounds and the energy flow from excited state species to the solvent

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Atomic-scale Materials Design, Lund University, University of Copenhagen
Authors: Kjær, K. (Ekstern), Haldrup, K. (Intern), Brandt van Driel, T. (Intern), Harlang, T. (Ekstern), Dohn, A. O. (Intern), Nielsen, M. M. (Intern)
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Conference: 245th National Spring Meeting of the American-Chemical-Society, New Orleans, LA, United States, 07/04/2013 - 07/04/2013
Main Research Area: Technical/natural sciences

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Volume: 245
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Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.101 SNIP 0
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.101 SNIP 0
Scopus rating (2006): SJR 0.101
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.104 SNIP 0.028
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.111 SNIP 0.008
Scopus rating (2002): SJR 0.115 SNIP 0.046
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.111 SNIP 0.038
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.111
Original language: English
Publication: Research - peer-review > Conference abstract in journal – Annual report year: 2013

Femtosecond X-ray Absorption Spectroscopy at a Hard X-ray Free Electron Laser: Application to Spin Crossover Dynamics

X-ray free electron lasers (XFELs) deliver short (<100 fs) and intense (similar to 10^(12) photons) pulses of hard X-rays, making them excellent sources for time-resolved studies. Here we show that, despite the inherent instabilities of current (SASE based) XFELs, they can be used for measuring high-quality X-ray absorption data and we report femtosecond time-resolved X-ray absorption near-edge spectroscopy (XANES) measurements of a spin-crossover system, iron(II) tris(2,2′-bipyridine) in water. The data indicate that the low-spin to high-spin transition can be modeled by single-exponential kinetics convoluted with the overall time resolution. The resulting time constant is similar to 160 fs.

General information
Glassy low-energy spin fluctuations and anisotropy gap in La$_{1.88}$Sr$_{0.12}$CuO$_4$

We present high-resolution triple-axis neutron scattering studies of the high-temperature superconductor La$_{1.88}$Sr$_{0.12}$CuO$_4$ ($T_c = 27$ K). The temperature dependence of the low-energy incommensurate magnetic fluctuations reveals distinctly glassy features. The glassiness is confirmed by the difference between the ordering temperature $T_N \approx T_c$ inferred from elastic neutron scattering and the freezing temperature $T_f \approx 11$ K obtained from muon spin rotation studies. The magnetic field independence of the observed excitation spectrum as well as the observation of a partial suppression of magnetic spectral weight below 0.75 meV for temperatures smaller than $T_f$ indicate that the stripe frozen state is capable of supporting a spin anisotropy gap, of a magnitude similar to that observed in the spin and charge stripe-ordered ground state of La$_{1.88}$Sr$_{0.12}$CuO$_4$. The difference between $T_N$ and $T_f$ implies that the significant enhancement in a magnetic field of nominally elastic incommensurate scattering is caused by strictly inelastic scattering—at least in the temperature range between $T_f$ and $T_c$—which is not resolved in the present experiment. Combining the results obtained from our study of La$_{1.88}$Sr$_{0.12}$CuO$_4$ with a critical reappraisal of published neutron scattering work on samples with chemical composition close to $p = 0.12$, where local probes indicate a sharp maximum in $T_f(p)$, we arrive at the view that the low-energy fluctuations are strongly dependent on composition in this regime, with anisotropy gaps dominating only sufficiently close to $p = 0.12$ and superconducting spin gaps dominating elsewhere.
Industriens udnyttelse af de store internationale Røntgen og neutron facilitter

Original language: Danish

Publisher: Dansk Metallurgisk Selskab
Main Research Area: Technical/natural sciences

Electronic versions: Vm_bogen_2013.pdf

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Publication: Research › Sound/Visual production (digital) – Annual report year: 2013
Interfacing MCNPX and McStas for simulation of neutron transport

Simulations of target-moderator-reflector system at spallation sources are conventionally carried out using Monte Carlo codes such as MCNPX[1] or FLUKA[2, 3] whereas simulations of neutron transport from the moderator and the instrument response are performed by neutron ray tracing codes such as McStas[4, 5, 6, 7]. The coupling between the two simulation suites typically consists of providing analytical fits of MCNPX neutron spectra to McStas. This method is generally successful but has limitations, as it e.g. does not allow for re-entry of neutrons into the MCNPX regime. Previous work to resolve such shortcomings includes the introduction of McStas inspired supermirrors in MCNPX. In the present paper different approaches to interface MCNPX and McStas are presented and applied to a simple test case. The direct coupling between MCNPX and McStas allows for more accurate simulations of e.g. complex moderator geometries, backgrounds, interference between beam-lines as well as shielding requirements along the neutron guides.

General information
State: Published
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Paul Scherrer Institut, Oak Ridge National Laboratory
Authors: Klinkby, E. B. (Intern), Lauritzen, B. (Intern), Nonbøl, E. (Intern), Willendrup, P. K. (Intern), Filges, U. (Ekstern), Wohlmuther, M. (Ekstern), Gallmeier, F. X. (Ekstern)
Pages: 106-110
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Main Research Area: Technical/natural sciences

Publication information
Volume: 700
ISSN (Print): 0168-9002
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.916 SNIP 1.352
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.915 SNIP 1.334 CiteScore 1.21
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.852 SNIP 1.303 CiteScore 1.24
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.944 SNIP 1.398 CiteScore 1.48
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.806 SNIP 1.071 CiteScore 1.19
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.918 SNIP 1.424 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.893 SNIP 1.113
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.75 SNIP 1.386
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Introducing a standard method for experimental determination of the solvent response in laser pump, x-ray probe time-resolved wide-angle x-ray scattering experiments on systems in solution

In time-resolved laser pump, X-ray probe wide-angle X-ray scattering experiments on systems in solution the structural response of the system is accompanied by a solvent response. The solvent response is caused by reorganization of the bulk solvent following the laser pump event, and in order to extract the structural information of the solute, the solvent response has to be treated. Methodologies capable of doing so include both theoretical modelling and experimental determination of the solvent response. In the work presented here, we have investigated how to obtain a reproducible solvent response—the solvent term—experimentally when applying laser pump, X-ray probe time-resolved wide-angle X-ray scattering. The solvent term describes difference scattering arising from the structural response of the solvent to changes in the hydrodynamic parameters: pressure, temperature and density. We present results based on NIR and dye mediated solvent heating, and demonstrate that the solvent response is independent of the heating method. The NIR heating is shown to be rendered unusable by higher order effects under certain experimental conditions, while the dye mediated solvent heating is demonstrated to exhibit first order behaviour with respect to the amount of energy deposited in the solution. We introduce a standardized method for recording solvent responses in laser pump, X-ray probe time-resolved X-ray wide-angle scattering experiments by using dye mediated solvent heating. Furthermore, we have generated a library of solvent terms, which can be used to describe the solvent term in any TRWAXS experiment, and made it available online.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, European Synchrotron Radiation Facility, Université de Rennes, University of Copenhagen
Authors: Kjær, K. S. (Intern), Brandt van Driel, T. (Intern), Kehres, J. (Intern), Haldrup, M. K. (Intern), Khakhulin, D. (Ekstern), Bechgaard, K. (Ekstern), Cammarata, M. (Ekstern), Wulff, M. (Ekstern), Sørensen, T. J. (Ekstern), Nielsen, M. M. (Intern)
Pages: 15003-15016
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 15
Issue number: 36
Manufacturing and Characterization of Silicon Compound Refractive Lenses for Focussing of Hard X-Rays

General information
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Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
Number of pages: 1
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Event: Abstract from 22nd International Congress on X-Ray Optics and Microanalysis, Hamburg, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract - Poster Contribution - Stöhr et. al..pdf

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Poster abstract
Source: dtu
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Microstructure, texture and magnetic properties of Ni-Cu-W substrates for coated conductors
The microstructure, texture, hardness and magnetization have been investigated in a series of strongly cube-textured (Ni95W5)100-xCux samples with x=0, 5, 10 and 15 at% Cu. It is found that the addition of 5 at% Cu to the Ni-5 at% W alloy results in a substantial decrease of the Curie temperature and in a reduction of the saturation magnetization without significant modification of the microstructure and the texture. This additionally alloyed material is only slightly softer than the Ni-5 at% W substrate. Although the Curie temperature and saturation magnetization decrease in the samples with higher concentrations of copper, increasing the Cu-content to 10 at% and 15 at% leads to increased frequencies of annealing twins in the cube-textured matrix. It is suggested that the (Ni 95W5)100-xCux alloy with x=5 at% Cu may be a good candidate material for using as a substrate for coated conductors. © 2012 Elsevier B.V.

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Wulff, A. C. (Intern), Mishin, O. (Intern), Andersen, N. H. (Intern), Yue, Z. (Intern), Grivel, J. (Intern)
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Main Research Area: Technical/natural sciences

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Journal: Materials Letters
Volume: 92
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Ratings:
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.757 SNIP 0.935
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.792 SNIP 1.021 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Optimization of cold neutron beam extraction at ESS

The present study takes its origin in the baseline design of European Spallation Source where a cold and a thermal moderator are situated next to each other enabling bispectral extraction. The study aims at mapping the differences in various neutron distributions depending on the angle and position from which the moderator is viewed. This study does not only show changes in both cold and thermal neutron flux, depending on extraction position, but also shows that there are significant differences in the wavelength spectrum and origin of neutrons depending on the angle of view.

General information
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB
Authors: Schönfeldt, T. (Intern), Batkov, K. (Ekstern), Klinkby, E. B. (Intern), Lauritzen, B. (Intern), Mezei, F. (Ekstern), Pitcher, E. (Ekstern), Takibayev, A. (Ekstern), Willendrup, P. K. (Intern), Zanini, L. (Ekstern)
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Optimization of neutron beam extraction at ESS

General information
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB
Authors: Schönfeldt, T. (Intern), Batkov, K. (Ekstern), Klinkby, E. B. (Intern), Lauritzen, B. (Intern), Mezei, F. (Ekstern), Pitcher, E. (Ekstern), Takibayev, A. (Ekstern), Willendrup, P. K. (Intern), Zanini, L. (Ekstern)
Number of pages: 1
Publication date: 2013
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Main Research Area: Technical/natural sciences
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Optimization_of_neutron_beam_poster.pdf
Links:
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Source: dtu
Source-ID: u::9813
Publication: Research - peer-review › Poster – Annual report year: 2013

Phase diagram with an enhanced spin-glass region of the mixed Ising-XY magnet LiHo_{x}Er_{1-x}F_{4}

We present the experimental phase diagram of LiHo_{x}Er_{1-x}F_{4}, a dilution series of dipolar-coupled model magnets. The phase diagram was determined using a combination of ac susceptibility and neutron scattering. Three unique phases in addition to the Ising ferromagnet LiHoF_{4} and the XY antiferromagnet LiErF_{4} have been identified. Below x=0.86, an embedded spin-glass phase is observed, where a spin glass exists within the ferromagnetic structure. Below x=0.57, an Ising spin glass is observed consisting of frozen needlelike clusters. For x∼0.3–0.1, an antiferromagnetically coupled spin glass occurs. A reduction of T_{C}(x) for the ferromagnet is observed which disobeyes the mean-field predictions that worked for LiHo_{x}Y_{1-x}F_{4}.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Institute of Physics, University of Bern, Helmholtz–Zentrum Berlin für Materialien und Energie
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Main Research Area: Technical/natural sciences
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Issue number: 1
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Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Preparation and characterization of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ thin films on MgO single crystal substrates by chemical solution deposition

Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ thin films have been deposited on MgO single crystal substrates by spin-coating a solution based on 2-ethylhexanoate precursors. Pyrolysis takes place between 200°C and 450°C and is accompanied by the release of 2-
ethylhexanoic acid, CO2 and H2O vapour. Highly c-axis oriented Bi2Sr2CaCu2O8 films were obtained after heat treatment at 840°C in air. The highest Tc of 81K was measured in a 10-layer film. Subsequent post-annealing in Ar and pure O2 did not improve the superconducting properties of the films and resulted in the appearance of Bi2CaCuO5 or Bi2(Sr, Ca)2CuO6 impurities.

General information
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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Institute of Chemical Technology
Authors: Grivel, J. (Intern), Kepa, K. (Intern), Hlásek, T. (Ekstern), Andersen, N. H. (Intern), Rubešová, K. (Ekstern)
Pages: 32-36
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
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Volume: 486
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.575 SNIP 0.924 CiteScore 1.14
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.446 SNIP 0.888 CiteScore 0.99
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.497 SNIP 0.83 CiteScore 0.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.439 SNIP 0.7 CiteScore 0.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.55 SNIP 0.621 CiteScore 0.79
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.652 SNIP 0.607 CiteScore 0.94
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.63 SNIP 0.631
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.412 SNIP 0.56
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.67 SNIP 0.576
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.532 SNIP 0.716
Scopus rating (2006): SJR 0.667 SNIP 0.556
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.793 SNIP 0.656
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.779 SNIP 0.644
Web of Science (2004): Indexed yes
Silicon Compound Refractive Lenses

General information
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Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
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Simulation of a suite of generic long-pulse neutron instruments to optimize the time structure of the European Spallation Source

We here describe the result of simulations of 15 generic neutron instruments for the long-pulsed European Spallation Source. All instruments have been simulated for 20 different settings of the source time structure, corresponding to pulse lengths between 1 ms and 2 ms; and repetition frequencies between 10 Hz and 25 Hz. The relative change in performance with time structure is given for each instrument, and an unweighted average is calculated. The performance of the instrument suite is proportional to (a) the peak flux and (b) the duty cycle to a power of approximately 0.3. This information is an important input to determining the best accelerator parameters. In addition, we find that in our simple guide systems, most neutrons reaching the sample originate from the central 3-5 cm of the moderator. This result can be used as an input in later optimization of the moderator design. We discuss the relevance and validity of defining a single figure-of-merit for a full facility and compare with evaluations of the individual instrument classes.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Ecole Polytechnique Federale de Lausanne (EPFL), European Spallation Source ESS AB, Institute for Energy Technology, University of Copenhagen
Authors: Lefmann, K. (Ekstern), Klena, K. H. (Ekstern), Birk, J. O. (Ekstern), Hansen, B. R. (Intern), Holm, S. L. (Ekstern), Bergbäck Knudsen, E. (Intern), Lieutenant, K. (Ekstern), von Moos, L. (Intern), Sales, M. (Ekstern), Willendrup, P. K. (Intern), Andersen, K. H. (Ekstern)
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Main Research Area: Technical/natural sciences
Publication information
Journal: Review of Scientific Instruments
Structure and Magnetic Properties of Cu₃Ni₂SbO₆ and Cu₃Co₂SbO₆ Delafossites with Honeycomb Lattices

The crystal structures of two Delafossites, Cu₃Ni₂SbO₆ and Cu₃Co₂SbO₆, are determined by high-resolution synchrotron powder X-ray diffraction. The Ni and Co are ordered with respect to Sb in the layer of edge sharing octahedra, forming magnetic layers with honeycomb geometry. High-resolution electron microscopy confirms ordering, and selected-area electron diffraction patterns identify examples of the stacking polytypes. Low temperature synthetic treatments result in disordered stacking of the layers, but heating just below their melting points results in nearly fully ordered stacking variants. The major variant in both cases is a monoclinic distortion of a 6-layer Delafossite polytype, but a significant amount of a 2-layer polytype is also present for the Ni case. The antiferromagnetic ordering with transitions, at 22.3 and 18.5 K for Ni and Co variants, respectively, is investigated by temperature and field dependent magnetization, as well as specific heat. The sharp magnetic transitions support the presence of well developed 2:1 ordering of the Co:Sb or Ni:Sb ions in the honeycomb layers. Neutron diffraction measurements at 4 K are used to determine the magnetic structures. For both the Ni and Co phases, the propagation vector is \( k = [100] \), and can be described as alternating ferromagnetic chains in the metal-oxide plane giving an overall antiferromagnetic “zigzag” alignment. While orientation of the magnetic moments of the Co is along the b-axis, the Ni moments are in the ac plane, approximately parallel to the stacking direction. Bulk magnetization properties are discussed in terms of their magnetic structures.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Princeton University, Max Planck Institute, Oak Ridge National Laboratory, Karlsruhe Institute of Technology KIT, Helmholtz–Zentrum Berlin für Materialien und Energie
Authors: Roudebush, J. H. (Ekstern), Andersen, N. H. (Intern), Ramlau, R. (Ekstern), Garlea, V. O. (Ekstern), Toft-Petersen, R. (Intern), Norby, P. (Intern), Schneider, R. (Ekstern), Hay, J. N. (Ekstern), Cava, R. J. (Ekstern)
Pages: 6083-6095
Publication date: 2013
Main Research Area: Technical/natural sciences
Studies on Directional Moderators for ESS

General information
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Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Los Alamos National Laboratory, European Spallation Source ESS AB, Indiana University-Purdue, Oak Ridge National Laboratory, ORNL
Authors: Zanini, L. (Ekstern), Baxter, D. (Ekstern), Batkov, K. (Ekstern), Gallmeier, F. X. (Ekstern), Iverson, E. (Ekstern), Klinkby, E. B. (Intern), Lauritzen, B. (Intern), Mezei, F. (Ekstern), Muehrer, G. (Ekstern), Nonbøl, E. (Intern), Schönfeldt, T. (Intern), Takibayev, A. (Ekstern), Willendrup, P. K. (Intern)
Number of pages: 1
Publication date: 2013
Event: Poster session presented at CRISP, Villigen, Switzerland.
Main Research Area: Technical/natural sciences
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Source-ID: 100890660
Publication: Research › Poster – Annual report year: 2014
Substrate decoration for improvement of current-carrying capabilities of YBa$_2$Cu$_3$O$_x$ thin films

The effects of substrate decoration with yttria and Y:ZrO$_2$ on the structural and electrical properties of the YBa$_2$Cu$_3$O$_x$ (YBCO) thin films are studied. The films were deposited on (LaAlO$_3$)$_3$–(Sr$_2$AlTaO$_8$)$_7$ substrates by pulsed laser deposition. Two different structures of decoration layer were applied, a template layer of nanoparticles and an uniform ultra-thin layer. Significant improvement of current-carrying capabilities was observed, especially at high external magnetic fields. Structural studies of these films reveal the presence of extended linear defects in the YBCO matrix. The formation of these structures is attributed to seeding of randomly oriented YBCO grains due to suppression of epitaxy in the very beginning of the deposition. The films of both kinds of decoration layers show nearly the same improvement of jC over the reference film at 77 and 50K: jC (5T and 50K) reaches 0.92 and 0.97MA/cm$^2$ for uniform and template decoration layers. At 5 and 20K the effect of template decoration layers is more beneficial: jC (5T and 20K) values are 3.5 and 4.1MA/cm$^2$, jC (5T and 5K) values are 6.4 and 7.9MA/cm$^2$, for uniform and template decoration layers, respectively.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Quantum Physics and Information Technology, Aveiro University, Technical University of Denmark
Authors: Khoryushin, A. (Intern), Mozhaev, P. (Intern), Mozhaeva, J. (Intern), Bdikin, I. K. (Ekstern), Zhao, Y. (Ekstern), Andersen, N. H. (Intern), Jacobsen, C. S. (Intern), Hansen, J. O. B. (Ekstern)
Pages: 1-8
Publication date: 2013
Main Research Area: Technical/natural sciences
The effects of excess yttria on the structural and electrical properties of the YBa2Cu3Ox (YBCO) thin films are studied. The films were deposited on (LaAlO3)0.3–(Sr2AlTaO8)0.7 substrates by pulsed laser ablation from targets with different elemental composition. An increase of yttrium content of the target leads to formation of porous films with significantly improved current-carrying capabilities. Structural studies of these films reveal presence of yttria nanoparticles embedded into the YBCO matrix. The highest obtained critical current density in an external magnetic field of 5T was 2.6MA/cm2 at 50K and 9.4MA/cm2 at 20K. The fabricated Y-enriched YBCO films remain c-oriented at least up to 600nm thickness with no significant suppression of the critical current density. © 2012 Elsevier B.V. All rights reserved.

Yttrium-enriched YBa2Cu3Ox thin films for coated conductors fabricated by pulsed laser deposition

The effects of excess yttria on the structural and electrical properties of the YBa2Cu3Ox (YBCO) thin films are studied. The films were deposited on (LaAlO3)0.3–(Sr2AlTaO8)0.7 substrates by pulsed laser ablation from targets with different elemental composition. An increase of yttrium content of the target leads to formation of porous films with significantly improved current-carrying capabilities. Structural studies of these films reveal presence of yttria nanoparticles embedded into the YBCO matrix. The highest obtained critical current density in an external magnetic field of 5T was 2.6MA/cm2 at 50K and 9.4MA/cm2 at 20K. The fabricated Y-enriched YBCO films remain c-oriented at least up to 600nm thickness with no significant suppression of the critical current density. © 2012 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Quantum Physics and Information Technology
Authors: Khoryushin, A. V. (Intern), Mozhaev, P. B. (Intern), Mozhaeva, J. E. (Intern), Andersen, N. H. (Intern), Grivel, J. (Intern), Hansen, J. O. B. (Ekstern), Jacobsen, C. S. (Intern)
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Scopus rating (2016): SJR 0.575 SNIP 0.924 CiteScore 1.14
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Scopus rating (2015): SJR 0.446 SNIP 0.888 CiteScore 0.99
BFI (2014): BFI-level 1
Air-stable π-conjugated amorphous copolymer field-effect transistors with high mobility of 0.3 cm²/Vs

We have fabricated organic bottom-contact top-gate field-effect transistors with an indenofluorene-phenanthrene copolymer semiconductor, exhibiting ON/OFF ratio of 10(7) and uncommonly high mobility for an amorphous conjugated polymer of up to 0.3 cm²/Vs. Lack of crystallinity in this material is indicated by atomic force microscopy, grazing incidence wide angle X-ray scattering, and differential scanning calorimetry data. Nevertheless, fitting transistor data to the Gaussian disorder model gives low energetic disorder of sigma = 48 meV and high prefactor mobility \(\mu(0) = 0.67\) cm²/Vs. The measured transistor mobility is also exceptionally stable in ambient conditions, decreasing only by approximately 15% over two months. (C) 2012 American Institute of Physics
An introduction to three-dimensional X-ray diffraction microscopy

Three-dimensional X-ray diffraction microscopy is a fast and nondestructive structural characterization technique aimed at studies of the individual crystalline elements (grains or subgrains) within millimetre-sized polycrystalline specimens. It is based on two principles: the use of highly penetrating hard X-rays from a synchrotron source and the application of tomographic reconstruction algorithms for the analysis of the diffraction data. In favourable cases, the position, morphology, phase and crystallographic orientation can be derived for up to 1000 elements simultaneously. For each grain its average strain tensor may also be derived, from which the type II stresses can be inferred. Furthermore, the dynamics of the individual elements can be monitored during typical processes such as deformation or annealing. A review of the field is provided, with a viewpoint from materials science. © 2012 International Union of Crystallography Printed in Singapore—all rights reserved.

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State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Poulsen, H. F. (Intern)
Pages: 1084-1097
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Scopus rating (2016): CiteScore 2.51 SJR 1.242 SNIP 1.234
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.322 SNIP 2.588 CiteScore 3.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.585 SNIP 4.371 CiteScore 4.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.921 SNIP 6.392 CiteScore 6
ISI indexed (2013): ISI indexed yes
Within the last decade a number of x-ray diffraction methods have been presented for non-destructive 3D characterization of polycrystalline materials. 3DXRD [1] and Diffraction Contrast Tomography [2,3,4] are examples of such methods providing full spatial and crystallographic information of the individual grains. Both methods rely on specially designed high-resolution near-field detectors for acquire the shape of the illuminated grains, and therefore the spatial resolution is for both methods limited by the resolution of the detector, currently ~2 micrometers. Applying these methods using conventional far-field detectors provides information on centre of mass, crystallographic orientation and stress state of the individual grains [5], at the expense of high spatial resolution. However, far-field detectors have much higher efficiency than near-field detectors, and as such are suitable for dynamic studies requiring high temporal resolution and set-ups involving bulky sample environments (e.g. furnaces, stress-rigs etc.)
Critical current density measurement of thin films by AC susceptibility based on the penetration parameter $h$

We have numerically proved that the dependence of AC susceptibility $\chi$ of a $E(J)$ power law superconducting thin disc on many parameters can be reduced to one penetration parameter $h$, with $E$ the electric field and $J$ the current density. Based on this result, we propose a way of measuring the critical current density $J_c$ of superconducting thin films by AC susceptibility. Compared with the normally used method based on the peak of the imaginary part, our method uses a much larger range of the AC susceptibility curve, thus allowing determination of the temperature ($T$) dependence of $J_c$ from a normally applied $\chi(T)$ measurement. A fitting equation $J_c=1.9Ha|\chi'|^{0.69/d}−0.4$.

General information
State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Wind Energy Systems, Neutrons and X-rays for Materials Physics
Authors: Li, X. (Ekstern), Grivel, J. (Intern), Abrahamsen, A. B. (Intern), Andersen, N. H. (Intern)
Pages: 6-14
Publication date: 2012
Main Research Area: Technical/natural sciences
This thesis presents the results of a study aimed at investigating important fabrication aspects of reel-to-reel processing of metal substrates for coated conductors and identifying a new substrate candidate material with improved magnetic properties. The effect of mechanical polishing on surface roughness and texture in Ni-5at.%W tapes in the cold-rolled condition was studied as a function of polishing grade. The surface roughness of the tape in the polished and annealed condition, and after subsequent coating with a Gd2Zr2O7 buer layer was investigated taking grain boundaries into account. It was observed that the initial mean surface roughness decreased after annealing except after very fine polishing. Additionally, the roughness of the buer layers were found to increase slightly for the fine polished substrates. Grain boundary grooving was observed to impose a lower limit for the mean surface roughness. Fractions of cube texture within deviations of 5° from the ideal cube orientation, in the annealed substrates, were found to be very sensitive to the surface roughness before annealing. Microstructure, texture, and topography were studied in a strongly cube-textured Ni-5at.%W substrate before and after an additional annealing (condition A1 and A2, respectively) simulating a buer layer crystallisation heat treatment. Condition A1 was characterised by a high fraction of cube texture, a high fraction of low angle grain boundaries and a low fraction of 3 boundaries. A strong correlation was observed between the grain boundary groove depth and boundary type. Coherent twin boundaries and low angle grain boundaries were characterised by the smallest average groove depth while significantly deeper grooves were observed at other boundary types. A similar correlation was observed between the inclination angle at groove walls and the boundary type. The microstructure was slightly coarser in condition A2 and it was accompanied by a cube texture strengthening and an increase in the fraction of low angle grain boundaries. The average depth of grain boundary grooves increased considerably at boundaries characterised by large misorientation angles, except for coherent twin boundaries. Significant changes were observed between the groove depth at stationary boundaries and a low fraction of 3 boundaries. A strong correlation was observed between the grain boundary groove depth and boundary type. Coherent twin boundaries and low angle grain boundaries were characterised by the smallest average groove depth while significantly deeper grooves were observed at other boundary types. A similar correlation was observed between the inclination angle at groove walls and the boundary type. The microstructure was slightly coarser in condition A2 and it was accompanied by a cube texture strengthening and an increase in the fraction of low angle grain boundaries. The average depth of grain boundary grooves increased considerably at boundaries characterised by large misorientation angles, except for coherent twin boundaries. Significant changes were observed between the groove depth at stationary boundaries which generally increased in depth and the grooves at migrating boundaries which typically became shallower compared to condition A1. Furthermore, migrating boundaries were found to abandon grooves and generate grooves at new positions. Despite the observed changes in the extent of grain boundary grooving, the mean surface roughness was almost identical before and after the additional annealing. Microstructure, texture, hardness and magnetic properties have been studied in a series of new Ni-Cu-W substrates. Adding 5 at.% copper to Ni-5at.%W was observed to substantially decrease the Curie temperature and saturation mass magnetisation values without significantly modifying the microstructure and texture compared with Ni-5at.%W. The hardness of this Ni-5Cu-5W substrate was only slightly less than the hardness of the reference Ni-5at.%W substrate. Further increasing the Cu-content was observed to result in a great decrease in the Curie temperature and saturation mass magnetisation values, but also a significant decrease in the fraction of cube texture and the fraction of low angle grain boundaries.
boundaries. Finally, a Ni-5Cu-5W substrate may be a good candidate material as a substrate in future coated conductors.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Wind Energy, Materials science and characterization
Authors: Wulff, A. C. (Intern), Grivel, J. (Intern), Andersen, N. H. (Intern), Mishin, O. (Intern)
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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Thesis_Wulff.pdf

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Ph.D. dissertation
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**Danish in-kind simulation efforts to the ESS - an overview**

**General information**
State: Published
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Klinkby, E. B. (Intern), Willendrup, P. K. (Intern), Lefmann, K. (Ekstern)
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**Magnetic phase diagram of magnetoelectric LiMnPO₄**
The nature of the spin-flop (SF) transition in the magnetoelectric quasi-2D Heisenberg system LiMnPO₄ is studied in fields applied along the a axis. A refinement of the magnetic structure using neutron diffraction data in the SF phase reveals that the spins reorient from being parallel to the a axis to be nearly along the c axis at magnetic fields between 4 and 4.7 T, depending on temperature. The low-field antiferromagnetic phase boundary is shown to join the spin-flop line tangentially at the so-called bicritical point, where there is a suppression of the ordering temperature. At the bicritical field, we observe an increased intensity of the Lorentz broadened elastic scattering at magnetic Bragg peaks above T_N as compared to zero field and 10 T, without an increase in peak width. This suggests an increased density of fluctuations at the bicritical field as compared to zero field.

**General information**
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Iowa State University, Paul Scherrer Institut, National Institute of Standards and Technology
Number of pages: 7
Pages: 224415
Molecular ordering of ethanol at the calcite surface

To produce biominerals, such as shells, bones, and teeth, living beings create organic compounds that control the growth of the solid phase. Investigating the atomic scale behavior of individual functional groups at the mineral-fluid interface provides fundamental information that is useful for constructing accurate predictive models for natural systems. Previous investigations of the activity of coccolith-associated polysaccharides (CAP) on calcite, using atomic force microscopy (AFM) [Henriksen, K., Young, J. R., Bown, P. R., and Stipp, S. L. S.Palentology 2004, 43 (Part 3), 725-743 ] and molecular dynamics (MD) modeling [ Yang, M., Stipp, S. L. S., and Harding, J. H.Cryst. Growth Des. 2008, 8 (11), 4066-4074 ], have suggested that OH functional groups control polysaccharide attachment. The purpose of this work was to characterize, using X-ray reflectivity (XR) combined with molecular dynamics (MD) simulations, the structuring on calcite of a layer of the simplest carbon chain molecule that contains an OH group, ethanol (CH 3-CH2-OH). We found evidence
that EtOH forms a highly ordered structure at the calcite surface, where the first layer molecules bond with calcite. The ethanol molecules stand up perpendicularly at the interface or nearly so. As a consequence, the fatty, CH3 ends form a new surface, about 6 Å from the termination of the bulk calcite, and beyond that, there is a thin gap where ethanol density is low. Following is a more disordered layer that is two to three ethanol molecules thick, about 14 Å, where density more resembles that of bulk liquid ethanol. The good agreement between theory and experiment gives confidence that a theoretical approach can offer information about behavior in more complex systems. © 2012 American Chemical Society.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Micro- and Nanotechnology, Theoretical Biophysics, University of Copenhagen
Authors: Pasarin, I. S. (Ekstern), Yang, M. (Ekstern), Bovet, N. E. (Forskerdatabase), Glyvradal, M. (Forskerdatabase), Nielsen, M. M. (Intern), Bohr, J. (Intern), Feidenhans'l, R. (Ekstern), Stipp, S. L. S. (Forskerdatabase)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.816 SNIP 1.391 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.895 SNIP 1.356 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.177 SNIP 1.382 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.051 SNIP 1.357 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.148 SNIP 1.4
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.156 SNIP 1.351
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.383 SNIP 1.34
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.449 SNIP 1.434
Web of Science (2007): Indexed yes
Non-destructive identification of micrometer-scale minerals and their position within a bulk sample

Using the conventional techniques of mineralogy, it has been a challenge to determine mineral identity, crystal orientation and spatial position of micrometer-sized crystals that are embedded in a rock, sediment or soil. Traditionally, the individual grains must be extracted and analyzed separately. Crushing or disintegrating a sample annihilates any possibility for gathering information from the texture of the porous media or the mineral assemblage close to the grains in question. A new method using three-dimensional X-ray diffraction (3DXRD) microscopy can be successfully applied to natural materials. We combined X-ray microtomography (XMT) and 3DXRD to investigate a sample of very fine-grained chalk containing fracture minerals. The XMT technique provides three-dimensional images of the particles and pore structure at very high resolution (350 nm voxel dimension) on samples less than 500 μm in diameter. The minor phases present as crystals in fractures were determined nondestructively with 3DXRD microscopy. The chalk fragment investigated is composed predominantly of randomly oriented nanometric crystals of calcite that produce powder rings where no texture can be observed. Superimposed on this pattern, Bragg diffraction peaks from the other crystalline phases were observed. Individual crystals of barite and pyrite only a few micrometers in diameter are present in the fractures. Magnetite, celestine and siderite, other minerals that might have been expected based on the XMT absorption contrast, were not identified. The crystal shape and in-fracture location, derived from the microtomograms, and the mineral identity, derived from 3DXRD, allowed us to propose that the fractures are original in these tiny drill cuttings; they were not induced by drilling and filled with drilling mud particles, thus allowing reliable estimates to be made of rock porosity and permeability.
The application of in-situ 3D X-ray diffraction in annealing experiments: First interpretation of substructure development in deformed NaCl

In-situ 3D X-ray diffraction (3DXRD) annealing experiments were conducted at the ID-11 beamline at the European Synchrotron Radiation Facility in Grenoble. This allowed us to nondestructively document and subsequently analyse the development of substructures during heating, without the influence of surface effects. A sample of deformed single crystal halite was heated to between 260-400 °C. Before and after heating a volume of 500 by 500 by 300 μm was mapped using a planar beam, which was translated over the sample volume at intervals of 5-10 μm in the vertical dimension. In the following we present partially reconstructed orientation maps over one layer before and after heating for 240 min at 260 °C. Additional small syn-heating "maps" over a constrained sample rotation of 12-30°. The purpose of this was to illuminate a few reflections from 1 or 2 subgrains and follow their evolution during heating. Preliminary results show that significant changes occurred within the sample volume, for which, surface effects can be excluded. Results show a number of processes, including: i) change in subgrain boundary misorientation angle and ii) subgrain subdivision into areas of similar lattice orientation with new subgrain boundary formation. These results demonstrate that 3DXRD coupled with in-situ...
heating is a successful non-destructive technique for examining real-time postdeformational annealing in strongly deformed crystalline materials with complicated microstructures. © (2012) Trans Tech Publications, Switzerland.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Stockholm University, Lund University, Universidad Autonoma de Barcelona, Eberhard-Karls-Universität Tübingen, Université Toulouse III - Paul Sabatier
Authors: Borthwick, V. (Ekstern), Schmidt, S. (Intern), Piazolo, S. (Ekstern), Gundlach, C. (Ekstern), Griera, A. (Ekstern), Bons, P. D. (Ekstern), Jessell, M. W. (Ekstern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.28 SJR 0.186 SNIP 0.306
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
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Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SNIP 0.342 SJR 0.235 CiteScore 0.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SNIP 0.467 SJR 0.279 CiteScore 0.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SNIP 0.419 SJR 0.247 CiteScore 0.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SNIP 0.406 SJR 0.271
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SNIP 0.389 SJR 0.343
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.297 SNIP 0.358
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.314 SNIP 0.5
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.37 SNIP 0.511
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.41 SNIP 0.56
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.449 SNIP 0.575
Web of Science (2004): Indexed yes
The three dimensional X-ray diffraction technique
This introductory tutorial describes the so called 3 dimensional X-ray diffraction (3DXRD) technique, which allows bulk non-destructive structural characterizations of crystalline materials. The motivations and history behind the development of this technique are described and its potentials are sketched. Examples of the use of the technique are given and future trends and developments are suggested. The primary aim of the paper is to give 3DXRD novices an easy introduction to the technique and to describe a way from a dream to reality and new results.
Towards a phase field model of the microstructural evolution of duplex steel with experimental verification

A phase field model to study the microstructural evolution of a polycrystalline dual-phase material with conserved phase fraction has been implemented, and 2D simulations have been performed. For 2D simulations, the model predicts the cubic growth well-known for diffusion-controlled systems. Some interphase boundaries are found to show a persistent non-constant curvature, which seems to be a feature of multi-phase materials. Finally, it is briefly outlined how this model is to be applied to investigate microstructural evolution in duplex steel. © (2012) Trans Tech Publications, Switzerland.

**General information**
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Northwestern University
Authors: Poulsen, S. O. (Intern), Voorhees, P. (Ekstern), Lauridsen, E. M. (Intern)
Pages: 635-642
Publication date: 2012
Conference: 4th International Conference on Recrystallization and Grain Growth, Sheffield, United Kingdom, 04/07/2010 - 04/07/2010
BFI conference series: International Conference on Recrystallization and Grain Growth (5010946)
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Materials Science Forum
Volume: 715-716
ISSN (Print): 0255-5476
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
X-ray diffraction contrast tomography (DCT) system, and an X-ray diffraction contrast tomography (DCT) method

Source: US2012008736A An X-ray diffraction contrast tomography system (DCT) comprising a laboratory X-ray source (2), a staging device (5) rotating a polycrystalline material sample in the direct path of the X-ray beam, a first X-ray detector (6) detecting the direct X-ray beam being transmitted through the crystalline material sample, a second X-ray detector (7) positioned between the staging device and the first X-ray detector for detecting diffracted X-ray beams, and a
processing device (15) for analysing detected values. The crystallographic grain orientation of the individual grain in the polycrystalline sample is determined based on the two-dimensional position of extinction spots and the associated angular position of the sample for a set of extinction spots pertaining to the individual grain.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Poulsen, H. F. (Intern), Lauridsen, E. M. (Intern)
Publication date: 2012

**Publication information**

Country: Denmark
IPC: G01N23/083
Patent number: WO2012003839
Date: 12/01/2012
Original language: English

**Bibliographical note**

DTU reference number: 92676-11
Main Research Area: Technical/natural sciences
Publication: Research › Patent – Annual report year: 2012

**Projects:**

*Development of a versatile slip-ring/rotary-union based in-operando high temperature functional material test cell for the DanMAX beamline*

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Neutrons and X-rays for Materials Physics
Period: 01/10/2017 → 31/03/2018
Number of participants: 3
X-ray synchrotron scattering
Acronym: Op-Stage
Project ID: DTU-029
Number of related Ph.D. students: 1
Project participant:
Karlsson, Maths (Ekstern)
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
Sierra Trujillo, José Xavier (Intern)

**Relations**

Related projects:
ESS & MAX IV: Cross border science and society
Project

**3D imaging center**

Department of Physics
Neutrons and X-rays for Materials Physics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Electrofunctional materials
Centre for oil and gas – DTU  
Period: 01/01/2016 → 01/01/2021  
Number of participants: 14  
Project participant:  
Dahl, Anders Bjorholm (Intern)  
Oddershede, Jette (Intern)  
Trinderup, Camilla Himmelstrup (Intern)  
Simonsen, Søren Bredmose (Intern)  
Zheng, Yi (Intern)  
Brink, Bastian (Intern)  
Lauridsen, Torsten (Ekstern)  
Thydén, Karl Tor Sune (Intern)  
Sanna, Simone (Intern)  
Baier, Sina (Intern)  
Bentzen, Janet Jonna (Intern)  
Christensen, Anders Nymark (Intern)  
Project Manager, organisational:  
Gundlach, Carsten (Intern)  
Project Manager, academic:  
Poulsen, Henning Friis (Intern)  

Relations  
Related projects:  
Alliance for Imaging and Modelling of Energy Applications  
Publications:  
Powder embossing method for selective loading of polymeric microcontainers with drug formulation  
Crack Tip Flipping under Mode I Tearing: Investigated by X-Ray Tomography  
In-Situ X-ray Tomography Study of Cement Exposed to CO2 Saturated Brine  
Graphite nodules in fatigue-tested cast iron characterized in 2D and 3D  
Scene reassembly after multimodal digitization and pipeline evaluation using photorealistic rendering  
From concept to in vivo testing: Microcontainers for oral drug delivery  
Synthesis and characterization of Fe–Ni/γ-Al2O3 egg-shell catalyst for H2 generation by ammonia decomposition  
Microstructure and micromechanics of the heart urchin test from X-ray tomography  
Surface Detection using Round Cut  
Characterization of graphite nodules in thick-walled ductile cast iron  
High-Performance Microchanneled Asymmetric Gd0.1Ce0.9O1.95-δ-La0.6Sr0.4FeO3-δ-Based Membranes for Oxygen Separation  

Characterisation and modelling of crystallographic orientation changes at the grain scale during plastic deformation  
Department of Mechanical Engineering  
Materials and Surface Engineering  
Department of Physics  
Neutrons and X-rays for Materials Physics  
Period: 01/04/2014 → 31/03/2017  
Number of participants: 3  
Project participant:  
Juul, Nicolai Ytterdal (Intern)  
Winther, Grethe (Intern)  
Oddershede, Jette (Intern)  

Relations  
Parent project:  
Multi-scale material models for smart metal forming
Related projects:
Mechanical and microstructural transients after strain path changes in metal forming

Multi-scale material models for smart metal forming
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

Department of Mechanical Engineering
Materials and Surface Engineering
Department of Physics
Neutrons and X-rays for Materials Physics
Manufacturing Engineering

DTU Admission Course
University of Illinois
Period: 01/02/2014 → 31/07/2017
Number of participants: 5
Acronym: MulMatMod
Number of related Ph.D. students: 2
Project participant:
Winther, Grethe (Intern)
Oddershede, Jette (Intern)
Bay, Niels Oluf (Intern)
Juul, Nicolai Ytterdal (Intern)
Jensen, Mikkel Ravn Boye (Intern)

Relations
Related projects:
Characterisation and modelling of crystallographic orientation changes at the grain scale during plastic deformation
Mechanical and microstructural transients after strain path changes in metal forming

Activities:
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity
Intragranular orientation spread induced by grain interaction
Grain-scale investigations of deformation and surface treatment of stainless steel
Deformation-induced intragranular orientation spread in ferrite investigated by 3DXRD and forward modeling
Combining crystal plasticity and dislocation theory to model dislocation boundary characteristics
Intragranular orientation spread induced by grain interaction
Analysis of grain-scale experimental data in a crystal plasticity framework
Measured Resolved Shear Stresses on Slip Systems in Austenitic Steel Grains

Publications:
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity
Deformation-induced orientation spread in individual bulk grains of an interstitial-free steel

Alliance for Imaging and Modelling of Energy Applications
The CINEMA research alliance will develop unique 3D micro-structural characterization methods, which make it possible to investigate components under realistic conditions and in real time. This will enable correlation between performance and local changes in the microstructure.

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Physics
Neutrons and X-rays for Materials Physics
Department of Wind Energy
Composites and Materials Mechanics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Scientific Computing
Mixed Conductors
Statistics and Data Analysis
University of Copenhagen
Northwestern University
University of Manchester
MaxLab
LM Wind Power
Haldor Topsoe AS
Xnovo Technology ApS
Rockwool International
Amminex Emissions Technology A/S
Period: 01/01/2014 → 31/12/2018
Number of participants: 26
Acronym: CINEMA
Project participant:
Mikkelsen, Lars Pilgaard (Intern)
Sørensen, Bent F. (Intern)
Bowen, Jacob R. (Intern)
Kuhn, Luise Theil (Intern)
Larsen, Rasmus (Intern)
Hansen, Per Christian (Intern)
Frandsen, Henrik Lund (Intern)
Gundlach, Carsten (Intern)
Dahl, Anders Bjorholm (Intern)
Yang, Shu-Yi (Intern)
Poulsen, Stefan Othmar (Intern)
Lyckegaard, Allan (Intern)
Lauridsen, Erik Mejdal (Intern)
Sørensen, Henning Osholm (Ekstern)
Project Manager, organisational:
Sørensen, Hanne (Intern)
Phd Student:
Jespersen, Kristine Munk (Intern)
Beil, Johannes (Ekstern)
Andersen, Michael (Intern)
Emerson, Monica Jane (Intern)
De Angelis, Salvatore (Intern)
Birkelund, Klaus (Ekstern)
Jacobsen, Hjalte Sylvest (Intern)
Chapelle, Lucie (Intern)
Supervisor:
Frandsen, Henrik Lund (Intern)
Project Manager, academic:
Andreasen, Jens Wenzel (Intern)
Project Coordinator:
Poulsen, Henning Friis (Intern)

Relations
Activities:
DTU Energy Conversion 2nd International PhD Summer School
Wilson K. S. Chiu
Gerardina Carbone

Publications:
High resolution ptychographic tomography of soft matter
3D X-Ray Computed Tomography (XCT) of Fatigue Damage Evolution in UD Glass Fibre Composite
Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging
Dictionary Based Segmentation in Volumes
Micromechanical Investigation of Fatigue Damage in Uni-Directional Fibre Composites
Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging
Fatigue damage evolution in fibre composites for wind turbine blades
Micromechanical Time-Lapse X-ray CT Study of Fatigue Damage in Uni-Directional Fibre Composites

FTP-PIEZO Multi-scale mapping of strain mechanisms in lead-free piezoceramics

Department of Physics
Neutrons and X-rays for Materials Physics

University of New South Wales
Period: 01/01/2013 → 14/03/2016
Number of participants: 3
Project participant:
Oddershede, Jette (Intern)
Schmidt, Søren (Intern)

Phd Student:
Majkut, Marta (Intern)

Relations
Related projects:
Multi-scale mapping of strain mechanisms in lead-free piezoceramics
Activities:
Quantitative grain-scale ferroelectric domain volume fractions and domain switching strains measured by 3DXRD during in situ electrical poling
Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying strain evolution in piezoelectric domain structures and deformation induced twinning
Materials characterisation tools towards lead-free piezoceramics

Publications:
Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction
The effect of inter-granular constraints on the response of polycrystalline piezoelectric ceramics at the surface and in the bulk
Maximising electro-mechanical response by minimising grain-scale strain heterogeneity in phase-change actuator ceramics
Heterogeneous grain-scale response in ferroic polycrystals under electric field
Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data
Activities:

**DANSCATT Annual meeting 2017**
Period: 2017
Martin Meedom Nielsen (Organizer)
Department of Physics
Neutrons and X-rays for Materials Physics

**Related event**

**DANSCATT Annual meeting 2017**
01/06/2017 → 02/06/2017
Odense, Denmark
Activity: Attending an event › Participating in or organising a conference

**Paul Scherrer Institut (External organisation)**
Period: Apr 2017
Martin Meedom Nielsen (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Swiss Light Source Proposal panel
Degree of recognition: International

**Related external organisation**

**Paul Scherrer Institut**
Switzerland
Activity: Membership › Membership in review committee

**Workshop for electromechanical and dielectric materials and devices**
Period: 9 Mar 2017
Astri Bjørnetun Haugen (Organizer)
Hugh Simons (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Department of Physics
Neutrons and X-rays for Materials Physics
Documents:
Workshop_poster

**Related event**

**Workshop for electromechanical and dielectric materials and devices**
09/03/2017 → ...
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany**
Period: 6 Oct 2016
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Address at the inauguration of the European XFEL Head Quarters

Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany

Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany

Related event

Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany
06/10/2016 → …
Schenefeld, Germany
Activity: Attending an event › Participating in or organising a conference

Intragranular orientation spread induced by grain interaction
Period: 12 Jul 2016
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

3rd International Congress on Materials Science
10/07/2016 → 13/07/2016
St. Charles, United States
Activity: Talks and presentations › Conference presentations

Mathematics Working Group of the European Society for Engineering Education (External organisation)
Mirza Karamehmedovic (Participant)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics

Description
National contact point for Denmark
Degree of recognition: International

Related external organisation

Mathematics Working Group of the European Society for Engineering Education
Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar

Chemical Dynamics in an X-ray Scattering Perspective
Period: 14 Jun 2016
Martin Meedom Nielsen (Keynote speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Research Opportunities in Photochemistry, Solar Energy & Advanced X-ray Methods
14/06/2016 → 17/06/2016
Menlo Park, United States
Activity: Talks and presentations › Conference presentations
Grain-scale investigations of deformation and surface treatment of stainless steel
Period: 8 Jun 2016
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
CHESS-U: New Industrial and Scientific Opportunities for Structural Materials: Data, Modeling, Manufacturing

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Fast Physical Processes studied at XFELs, Dynamic Structural Science Workshop, Cosener's House, Abingdon, UK
Period: 25 Apr 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Dynamic Structural Science Workshop
Oxford, United Kingdom
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

HD-Tomo Days
Period: 6 Apr 2016 → 8 Apr 2016
Mirza Karamahmedovic (Participant)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics

Description
HD-Tomo Days

Related event

HD-Tomo Days
06/04/2016 → 08/04/2016
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Electronic and Structural Dynamics in Solvated Metal Complexes Enlightened by XFEL Experiments, Workshop to Define the Science Case for a Soft X-ray Laser Beamline at MAX IV, Stockholm, SE
Period: 21 Mar 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Electronic and Structural Dynamics in Solvated Metal Complexes Enlightened by XFEL Experiments, Workshop to Define the Science Case for a Soft X-ray Laser Beamline at MAX IV, Stockholm, SE
21/03/2016 → 21/03/2016
Inverse scattering problems in characterisation of nanomaterials
Period: 11 Feb 2016
Mirza Karamahmedovic (Invited speaker)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics

Description
Inverse scattering problems in characterisation of nanomaterials
Degree of recognition: International

Related event

Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany
Period: 8 Feb 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany
Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany

Related event

European XFEL users meeting
Period: 27 Jan 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Opening Address, XFEL.EU users meeting, Hamburg, Germany.

Opening Address, XFEL.EU users meeting, Hamburg, Germany.

Related event

European XFEL users meeting
27/01/2016 → 29/01/2016
Hamburg, Germany
Materials characterisation tools towards lead-free piezoceramics
Period: 17 Dec 2015
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
DTU Sustain Conference 2015
17/12/2015 → 17/12/2015
Lyngby, Denmark

Quantitative grain-scale ferroelectric domain volume fractions and domain switching strains measured by 3DXRD during in situ electrical poling
Period: 1 Oct 2015
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
8th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation
30/09/2015 → 02/10/2015
Grenoble, France

Polymer injection molding of hard X-ray refractive optics
Period: 24 Sep 2015
Frederik Stöhr (Speaker)
DTU Danchip
Neutrons and X-rays for Materials Physics

Related event
41st International conference on Micro and Nano Engineering : MNE 2015
21/09/2015 → 24/09/2015
The Hague, Netherlands

23rd International Congress on X-ray Optics and Microanalysis
Period: 14 Sep 2015 → 15 Sep 2015
Frederik Stöhr (Participant)
DTU Danchip
Neutrons and X-rays for Materials Physics

Description
Poster Presentation
Microfabrication and testing of refractive hard X-ray optics

Related event
23rd International Congress on X-ray Optics and Microanalysis
14/09/2015 → 18/09/2015
Upton, New York, United States
Activity: Attending an event › Participating in or organising a conference

**MyFab-NorFab meeting 2015**
Period: 21 Apr 2015 → 22 Apr 2015
Frederik Stöhr (Participant)

DTU Danchip
Neutrons and X-rays for Materials Physics

**Description**
Poster presentation on recent progress in silicon hard X-ray lens development at DTU Danchip.

X-ray refractive optics. Manufacture, shape characterization and optical performance.

**Documents:**
Poster

**Links:**
http://www.myfab.se/Start/MyfabUserMeeting.aspx (Myfab and NorFab User Meeting 2015)

**Related event**

**MyFab-NorFab meeting 2015**
21/04/2015 → 22/04/2015
Lund, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Three-Dimensional X-ray Diffraction (3DXRD) microscopy for in situ studies of polycrystalline materials**
Period: 16 Mar 2015
Jette Oddershede (Lecturer)

Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Polycrystalline Materials: Bringing Together Experiments, Simulations, and Analytical Theories, invited presentation.

**Related event**

**TMS 2015 Annual Meeting & Exhibition**
15/03/2015 → 19/03/2015
Orlando, FL, United States
Activity: Talks and presentations › Conference presentations

**Chair of the Search and Selection Committee XFEL. EU (External organisation)**
Martin Meedom Nielsen (Chairman)

Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Chair of the Search and Selection Committee for the Chairperson of the Management Board, XFEL. EU
Degree of recognition: International

**Related external organisation**

**Chair of the Search and Selection Committee XFEL. EU**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**4th Annual Niels Bohr International Academy Workshop-School on ESS Science**
Period: 10 Nov 2014 → 14 Nov 2014
Ellen Fogh (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
This year our workshop-school is intended to be a forum of discussion of how the use of X-ray and neutron reflectometry tells us about the binding of molecules to a surface and of how the characteristic frequencies of motions of surface-bound molecules can be detected by inelastic neutron scattering, and finally, how such experimental results can be interpreted by molecular dynamics simulations.

Documents:
highFieldPoster

Related event

4th Annual Niels Bohr International Academy Workshop-School on ESS Science
10/11/2014 → 14/11/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Magnetic High-Field Phases of Magnetoelectric LiNiPO4
Period: 30 Oct 2014
Ellen Fogh (Speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
The scope of the workshop is to bring together experts doing research in high magnetic fields above 15 T with the focus on neutron scattering. We want to provide an information platform for researchers regarding the future use of the high-field facility capable to generate magnetic fields as high as 25+ T at HZB. Identification of possible future experiments using this facility is one of the main workshop topics. The workshop covers a broad field of topics ranging from the neutron diffraction and scattering in high magnetic fields and sample environment for neutron sciences up to fundamental physics problems in high magnetic fields.

Documents:
abstract_hfm_workshop_EllenFogh

Related event

Neutron Scattering in Magnetic Fields Above 15 Tesla
29/10/2014 → 30/10/2014
Berlin, Germany
Activity: Talks and presentations › Conference presentations

World Conference on Neutron Radiography
Alberto Cereser (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics
Documents:
Poster WCNR 2014

Related event

World Conference on Neutron Radiography
05/10/2014 → 10/10/2014
Grindewald, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying strain evolution in piezoelectric domain structures and deformation induced twinning
Period: 30 Sep 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Nordic X-ray Science Days
29/09/2014 → 01/10/2014
Lund, Sweden
Activity: Talks and presentations › Conference presentations

Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Period: 15 Jul 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Seminar at Department of Materials, University of Oxford, UK

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Chair of the Council of the European XFEL (External organisation)
Period: 1 Jul 2014 → 30 Jun 2018
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
The Council is the shareholders representation and, the supreme organ of the European XFEL.EU
Chair of the European XFEL Council, the supreme organ of the European XFEL.

Body type: Governing body
Degree of recognition: International

Related external organisation
Chair of the Council of the European XFEL
Deformation-induced intragranular orientation spread in ferrite investigated by 3DXRD and forward modeling
Period: 1 Jul 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
2nd International Congress on 3D Materials Science
29/06/2014 → 02/07/2014
Annecy, France
Activity: Talks and presentations › Conference presentations

Inverse scattering: from formulation to application
Period: 10 Mar 2014
Mirza Karamehmedovic (Invited speaker)
Department of Applied Mathematics and Computer Science
Scientific Computing
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
Lecture at International University of Sarajevo
10/03/2014 → …
Sarajevo, Bosnia and Herzegovina
Activity: Talks and presentations › Conference presentations

Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Period: 19 Feb 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Invited presentation

Related event
TMS 2014 143rd Annual Meeting and ExhibitionAnnual Meeting & ExhibitionAnnual Meeting & Exhibition2014
16/02/2014 → 20/02/2014
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Period: 25 Oct 2013
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
CLASSE seminar at the Cornell High Energy Synchrotron Source, CHESS, Cornell University, Ithaca NY, USA

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Period: 11 Sep 2013
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
7th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation
10/09/2013 → 12/09/2013
Sydney, Australia
Activity: Talks and presentations › Conference presentations

Local stress distributions studied at the single grain level
Period: 9 Oct 2012
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
9th Conference on Residual Stress
07/10/2012 → 10/10/2012
Garmisch-Partenkirchen, Germany
Activity: Talks and presentations › Conference presentations

Measuring Grain Resolved Stresses during in situ Plastic Deformation using 3DXRD
Period: 6 Jan 2012
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Invited presentation
Documents:
Oddershede_3page_revised

Related event
International Symposium on Plasticity 2012 and Its Current Applications
03/01/2012 → 08/01/2012
San Juan, Puerto Rico
Activity: Talks and presentations › Conference presentations

European XFEL (External organisation)
Period: 1 Jun 2011 → 30 Jun 2014
Martin Meedom Nielsen (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Delegate to the Council of the European XFEL, appointed by DASTI
Delegate to the Council of the European XFEL, appointed by DASTI
Body type: Governing Body
Degree of recognition: International

Related external organisation
European XFEL
Germany
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Press clippings:

Dansk professor får prestigefuld toppost i Hamborg
Martin Meedom Nielsen
17/10/2016
Department of Physics, Neutrons and X-rays for Materials Physics

Media contribution (1)

Dansk professor får prestigefuld toppost i Hamborg
17/10/2016
Uddannelses og Forskningsministeriet, Web
http://ufm.dk/aktuelt/nyheder/2016/dansk-professor-far-prestigefuld-toppost-i-hamborg
Martin Meedom Nielsen
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Press / Media

Der beste Laser der Welt
Martin Meedom Nielsen
06/10/2016
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Media contribution (1)

Der beste Laser der Welt
06/10/2016
Die Zeit, Print
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