Self-Assembly of Metallic Supercrystals

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The design of nanomaterials with new structural properties is a wide application field for Small Angle Scattering (SAS) techniques. Many nanomaterials are relying on the self-assembly of metallic nanoparticles. Thanks to recent progresses in nanochemistry, metallic nanoparticles with controlled shape and size can be synthesized in large quantities and can be self-assembled into supercrystals using slow drying, depletion interactions or magnetic forces. Such metallic nanoparticles act as super-atoms that can crystallize together leading to periodic supercrystals as well as quasiperodic ones.

Shapes of particular interest are Platonic solids like cube, octahedron, tetrahedron as well as anisotropic shapes like faceted pentagonal rods or triangular platelets. As a result, a rich palet of polyhedral shapes for metallic nanoparticles is now available experimentally and we will discuss the current challenges in the SAS modeling of form factors as a powerful strategy for their characterization.
Crystallography has to be adapted to these faceted and possibly anisotropic solid shapes and some geometrical rules can help predicting optimal packings. We will give recent examples of supercrystals, including polymorphism of pentagonal nanorods and binary mixtures of Platonic solids.

What a Mess: Unraveling Structural Disorder in Battery Electrodes

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The functionality of rechargeable ion batteries is largely governed by the ability of the electrodes to store and transport electrons and active ions, such as Li-ions in Li-ion batteries. The efficiency and reversibility of these processes depend on the nature of the structural transformations accompanying charge and discharge. To fully understand these transformations, it is essential to study them under conditions that mimic real battery operation, using operando techniques.

Historically, research has focused on the crystalline structures of electrode materials, often employing only diffraction methods. However, a growing body of evidence shows that ion intercalation can also induce severe structural disorder ranging from defect formation to complete amorphization.

In this talk, I will present our work on integrating operando synchrotron X-ray absorption spectroscopy, diffraction, and total scattering to track the structural evolution in battery electrode materials as they undergo varying degrees of disorder during cycling. The talk will center on new layered $NaMO_2$ (M = transition metal) electrodes for Na-ion batteries. Additionally, I will discuss our recent findings on beam damage during operando synchrotron experiments, which have important implications for the accurate characterization of battery materials.

Operando mapping of morphology, phase transformations, and current patterns in energy devices by time-of-flight neutron diffraction and polarised neutron imaging

Luise Theil Kuhn

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A core activity in the ESS Lighthouse Hard Materials in 3D, SOLID (https://solid.dtu.dk/), has been to develop advanced neutron imaging methods for operando analysis of microstructure, phase transformations, and current patterns in energy devices. Here, I will present two cases where we have investigated the battery cell degradation of Na-ion batteries while being charged and discharged, and the current pattern formation in a proton exchange membrane water electrolysis (PEMWE) cell under operation.

Na-ion batteries are one of the promising next-generation battery technologies since they can deliver a capacity comparable to Li-ion batteries while constituting cheap, non-flammable, and sustainable materials. However, the chemical and mechanical stability during cycling is a challenge. The Na-ion battery is inherently difficult to directly image as Na has a very low X-ray and neutron scattering cross-section and can't sustain post-mortem disassembly and analysis. At the SENJU beamline at J-PARC, we have successfully performed the first multimodal operando neutron studies combining time-of-flight diffraction and Bragg edge imaging to investigate the microstructural changes and phase transformations of the battery electrodes and link them to the electrochemically active regions.

PEMWE cells are considered one of the key technologies for sustainable hydrogen production. PEMWE can be operated under relatively flexible conditions, making them ideal for varying electricity production by e.g. wind turbines or solar cells. A central component is the porous transport layer (PTL), which is used for managing the distribution of water and release of produced gasses. The PTL is subject to a very harsh environment and is often based on Ti coated with Pt or Ir. The morphology of the PTL is crucial for the performance of the PEMWE since this is directly linked to the oxygen bubble formation and the current pattern formation in the cell. At the RADEN beamline at J-PARC and NeXT at ILL, we have performed the first polarised neutron imaging studies of the current pattern formation in the PEMWE cell under operation while linking it to the electrochemical performance with different types of PTLs.

Neutrons in a haystack: Approaching small-angle scattering at ESS

Oliver Hammond
ESS-DMSC

Small-angle neutron scattering (SANS) is a key technique for non-destructive measurements of nanometre-to-micron scale structure, enabling insight into hierarchical organization in soft matter, life sciences, and functional materials. Its broad applicability makes it a key part of the European Spallation Source (ESS) instrumentation strategy, with SANS capabilities planned across multiple beamlines and divisions.[1]

This contribution focuses on LoKI, a broadband SANS instrument in the ESS Tranche 1 portfolio. LoKI will exploit the high time-averaged flux of the ESS source, enabling highthroughput measurements, smaller beam footprints, and enhanced flexibility in sample environments. We present an overview of current progress towards LoKI's user readiness, with emphasis on data-centric workflows within the remit of the ESS Data Management & Software Centre (DMSC). In particular, we highlight the integration of *Scipp*, an open-source Python library designed for efficient, interactive manipulation of multidimensional datasets within Jupyter environments.[2] We describe the development of modular, widget-based reduction workflows and real-time visualization capabilities tailored for LoKI's $^{10}B_4C$ straw tube detectors, supporting both standard SANS measurements and time-resolved applications.

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Unravelling the crystal structures of Ag_2Ch (Ch = S, Se, Te) from simultaneous powder X-ray diffraction and total scattering

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The binary silver chalcogenides Ag_2Ch (Ch = S, Se, Te) have in recent years become attractive candidates for low- to medium-temperature thermoelectric materials[1–3] with compositions based on Ag_2S even displaying metal-like ductility.[4] While understanding the structural features of the Ag_2Ch compounds that facilitate their properties is highly desirable, such analysis is currently limited by a poor understanding of their crystal structures. By collecting simultaneous synchrotron powder X-ray diffraction and total scattering, average structures determined from Rietveld refinement and maximum-entropy method (MEM) modelling are compared to the pair-distribution functions (PDFs). The Rietveld models at high temperature struggled to resolve the Ag substructure which is highly diffuse. A more accurate representation of the average structure can be derived from model-free MEM analysis; however, accurate estimation of the observed intensities is difficult due to the emergence of intense diffuse scattering at high temperature. The diffuse scattering indicates considerable disorder which the average structure cannot resolve. The result is an incorrect description of the local order which is also a problem for the room-temperature structures. From these observations, a new picture for understanding the correlated disorder in Ag_2Ch is proposed.

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Neutron studies of $SrCu_2(BO_3)_2$ under extreme conditions – a fruit fly for quantum many body physics

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Neutron spectroscopy offer a unique insight into the emergent quantum phases and entangled dynamics in quantum materials. A textbook example is offered by the compound SrCu2(BO3)2 realizing the Shastry-Sutherland model, which reveal a plethora of intriguing phenomena including: bosonic flat bands; a zoo of entangled bound states; correlated decay of magnons; valence bond solid of plaquette singlets; a quantum equivalent to the critical point of water; a putative deconfined quantum critical point; fractional magnetization plateaus and bosonic BEC of triplet bound states. Exploring this rich physics illustrates the challenges and rewards of technological advancements in neutron instrumentation and pushing the capabilities of extreme condition sample environments.

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Insights into molecular pharmacology from time-resolved structural biology at synchrotrons and X-ray free electron lasers

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Structural biology is critical for understanding how proteins work on the molecular level. However, resolving the temporal evolution of biological macromolecules in response to stimuli—such as the binding and release of small molecular ligands or drug molecules—remains a challenge. In recent years, our research group has leveraged synchrotron and X-ray free electron laser facilities to experimentally investigate how rhodopsins, acting as pumps, channels, or light sensors, are activated at the atomic level across time scales ranging from femtoseconds to milliseconds.

In our latest experiments, we explored how photoactive azobenzene compounds can be used to trigger protein dynamics for structural studies. My presentation will focus on the dissociation dynamics of the photopharmacological drug candidate azo-combretastatin A4 from tubulin, capturing events from the initial photochemical reaction through the disruption of high-affinity protein-ligand interactions, adaptation of the binding pocket, and the eventual release of the compound. I will discuss the relevance of these findings for our understanding of how anti-cancer drugs destabilize the microtubule network. Furthermore, I will present how light-switchable caffeine and beta-blocker derivatives can be used to track the dynamic plasticity of the ligand binding pocket in prototypical G protein-coupled receptors.

Search for loop currents in CsV_3Sb_5 with neutron spectroscopy and spin-ARPES

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Discovered in 2019, the AV_3Sb_5 (A = K, Rb, Cs) family of superconductors has attracted significant attention due to its intriguing kagome lattice structure, which offers a unique platform for exploring exotic physical phenomena. Most intriguing is the potential emergence of loop currents, which would give rise to weak magnetism.

We have used neutron spectroscopy to look for the excitations that would be associated with loop current magnetism. The sample is a 815 mg mosaic of 31 smaller crystals co-aligned in the HK scattering plane, with a mosaic spread of $\sim 2^\circ$. We present data from the thermal triple-axis spectrometer IN20 at the Institut Laue-Langevin and from the cold spectrometer CAMEA at the Paul Scherrer Institute covering the energy transfer range $\hbar\omega = 0.5$ - 12 meV. We find no evidence for magnetic excitations in CsV_3Sb_5 neither below nor above the superconducting temperature of T_C=2.5 K. We normalize to absolute units, $S(\boldsymbol{Q},\omega)g^2|f^2(\boldsymbol{Q})|$, and employ a simple spin dynamics model to place an upper limit on the magnetic moment from potential loop currents. This result, is enriched by our spin- and angle-resolved photoemission spectroscopy measurements, which also show an overall time-reversal symmetry conserved situation. However, by using the combination of spin-detection and circular dichroism, we are able to measure finite hidden quantities, reminiscent of similar topologically nontrivial sister-compounds.

* These authors contributed equally to this work.

Operando study of degradation and sodium storage process in sodium-ion batteries

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We present neutron powder diffraction and Bragg-edge imaging as a multi-modal method to investigate battery functioning in operando. The high neutron attenuation of lithium allows tracking battery operation by visualizing lithium diffusion processes. This is useful in battery studies, because it is a good way to determine which parts of the electrode under investigation are properly functioning, and which are not. This type of investigation is not as easy for sodium batteries, due to the lower attenuation of Na-ions, compared to Li-ions. To be able to track sodium diffusion processes with an imaging method, another approach is required. Bragg-edge imaging, relying on coherent scattering from the Na ions, allows us to spatially visualize crystallographic information, providing us with a way to track diffusion processes in a similar manner as in lithium-ion batteries. A Bragg-edge pattern consists of a plot of attenuation against wavelength. When satisfying the Bragg diffraction conditions dips are observed in transmission mode at lambda=2*d for various lattice planes in the crystalline phase. By acquiring such a type of signal pixel-by-pixel, we obtain spatially resolved crystallographic information, providing us with the ability to track phase change in operando. As a result, we can track battery operation as the electrode material under investigation undergoes phase-transition throughout a cycling process. The measurement was performed at SENJU@J-PARC, while relying on the SENJU banks as diffraction detectors, and the LumaCam detector as transmission detector for energy-resolved imaging. By combining the LumaCam with a diffraction detector, it was possible to validate the result of the spatially resolved detector, while also obtaining high-resolution global information on the sample through diffraction. Consequently, active and inactive areas of the electrode could be identified by tracking the phase transition process of the Prussian white electrode.

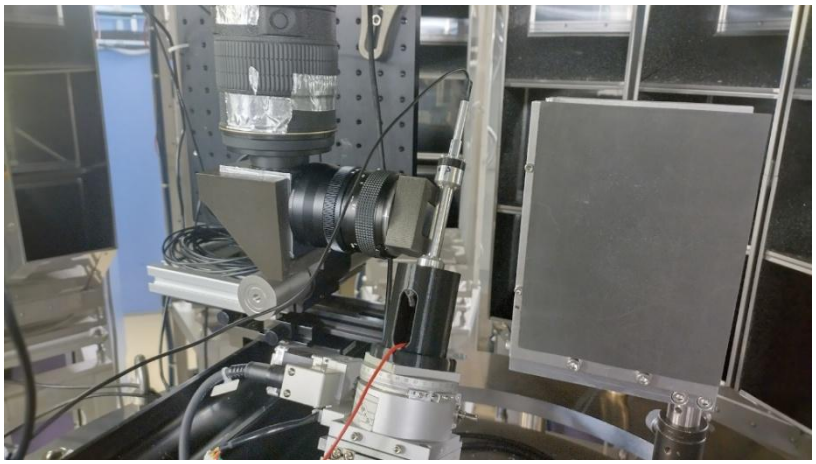

Figure 1. Experimental setup at SENJU@J-PARC.

Operando Diffraction for H_2 Production – the Reversible Memory Reactor

John S.O. Evans[a]

Abstract. The water-gas shift reaction (WGS, CO + H_2O ⇋ CO_2 + H_2) is a crucial step in the production of H_2 gas. It is performed on a multimillion-ton scale annually, often as a follow on to steam methane reforming (SMR; CH_4 + H_2O ⇋ CO + $3H_2$,) to increase hydrogen yield. The reverse reaction is of equal potential importance in CO_2 capture and its conversion to useful chemical building blocks. The equilibrium constant (K_{eq}) of WGS at the temperature where one might like to work for rapid kinetics and for integration with SMR is $K_{eq} \approx 1.0$ (T = 820 C), which means the reaction is inherently inefficient – only 50% of the reactants are converted to products, and significant energy would be needed to separate the mixed gas product stream.

In this talk I'll discuss how the defect chemistry of perovskite $ABO_{3-\delta}$ "oxygen carrier materials" (OCMS) in equilibrium with counter flows of the reactive CO and H_2O gases can be used to design a "Memory Reactor". Remarkably, this reactor allows one to "beat" chemical equilibrium limitations and perform the WGS reaction at close-to-100% conversion (super-equilibrium operation). In addition, the design produces naturally separated streams of H_2 and CO_2 product gases, removing the need for subsequent purification. I'll discuss how in situ and operando powder diffraction studies have allowed us to study the chemistry of the perovskite oxygen carrier material, prove the method of operation of the reactor, and test the range of conditions under which it can be operated reversibly. Time permitting, I'll also discuss the development of new OCMs, how the reactor can be used for other important reactions, and ex-situ experiments to study the local structure of OCM materials.

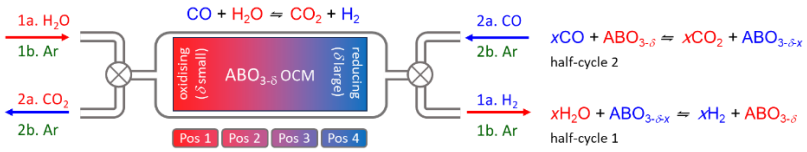

FIGURE 1. A schematic view of the Memory reactor. Pure H_2 gas is produced in half-cycle 1a and pure CO_2 in half-cycle 2a.

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Software and Science at the European Spallation Source

Henrik Jacobsen
ESS-DMSC

The European Spallation Source (ESS) is nearing the start of operations and is poised to become the world's brightest neutron source. With this leap in capability comes a corresponding increase in data volume and complexity. The Data Management and Software Centre (DMSC) plays a critical role in enabling scientific discovery at ESS by providing the software infrastructure that supports the entire experimental workflow—from instrument control to data reduction, visualization, and analysis.

In the first part of this talk, I will present some of the key software tools developed at DMSC and demonstrate how they help users efficiently transform raw neutron data into scientific results.

In the second part, I will shift focus to my own research on antiferromagnetic spintronic materials. These systems are of growing interest for their potential in next-generation information technologies, and ESS will provide unique insights into their fundamental properties.

Unraveling the hierarchical structure of narwhal tusk

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Keywords: Mineralized tissue; Narwhals; Scattering/Diffraction; Hierarchical materials;

Narwhals are fascinating animals whose left-handed spiral tusk has caught the attention of humankind for centuries and has been associated with the unicorn myth. The twisted tusk, which grows principally in males, has highly anisotropic mechanical properties and an extraordinarily high impact resistance [1]. We hypothesize that the orientation of the biological nanostructure reflects the spiral macro-structure, which defines the mechanical properties.

We combined 2D and 3D imaging techniques using X-rays and polarized visible light to study its hierarchical structure at multiple length scales. Small-angle X-ray scattering and diffraction imaging [3], X-ray fluorescence, and birefringence microscopy were used to investigate the anisotropy of the tusk building blocks (i.e., mineralized collagen fibrils) from the nano to the macro scale.

Narwhal tusks have a central pulp chamber surrounded by primary dentine and a layer of cementum. Unlike human teeth, no enamel is present [2]. The building blocks of the narwhal cementum and dentine are identical to other mineralized tissues; however, their degree of anisotropy and spatial distribution differ from, e.g., bone [4]. SAXS tensor tomography revealed a strong anisotropy in the dentine with mineralized collagen aligned in the longitudinal direction. A twist in the orientation of the longitudinal fibers was also found with radially increasing angles, creating a helical pattern from the pulp chamber to the cementum layer. The outer cementum layer that covers the entire tusk had a less anisotropic structure with radially oriented domains embedded in a longitudinally oriented matrix. At the nanoscale, the periodicity of the collagen fibrils was slightly higher in cementum than in dentine. The shape and size of the mineral particles were estimated fitting the SAXS and WAXS patterns, where the particle thickness and length increased from the inner to the outer dentine.

These results not only reveal that strong anisotropy is present at multiple scales in narwhal tusk tissue but also suggest that they follow a three-dimensional spiral structure in the nanoscale. The combination of 2D and 3D imaging techniques achieved an optimal balance between field of view, measurement time, and resolution at multiple length scales.

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MicroMAX – a beamline with time-resolved macromolecular crystallography capabilities at the MAX IV Laboratory

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The rise of 4th generation sources, including the MAX IV Laboratory 3 GeV ring, has enabled new possibilities to study dynamics using crystallography. The MicroMAX beamline is focussed on providing optimal X-ray characteristics for serial and time-resolved crystallography. The beamline offers a flexible sample environment for bespoke experimental setups and supports also high-throughput single crystal data collections.

MicroMAX recently started user operations and has performed experiments with SPINE-based fixed targets, flow injectors (high viscosity extrusion, capillary), and customized microfluidics mounted to an MD3-up diffractometer. Time-resolved SSX measurements have also been performed using a nanosecond pump laser (210-2600 nm). An X-ray chopper (0,8-70% duty cycle) in conjunction with a Jungfrau 9M Si integrating hybrid pixel detector also enables 2 kHz data collections at 10 μs resolution. Data can also be collected with an Eiger2 X 9M CdTe photon counting hybrid pixel detector, with automatic changes between both detectors in under a minute. The end station is equipped with an automatic sample changer (ISARA2) that can be used in cryogenic conditions housing up to 29 unipucks but can also exchange crystallisation plates and room-temperature spine-based sample holders. Experiments are controlled by MXCuBE with ISPyB used for data management. Automated fast feedback is implemented as well as data processing using CrystFEL.

The second experimental hutch at MicroMAX can be used for other activities while the first hutch is in X-ray operation. The second hutch is currently used as an off-line laser and spectroscopy laboratory for sample pre-characterization studies but will later be available for X-ray experiments.

The beamline has two monochromators, a crystal monochromator giving a narrow bandwidth beam with up to 10^{13} photons/s and a multilayer monochromator giving a wider bandwidth (up to 1%) with more than 10^{14} photons/s. The X-ray beam is initially focused by beryllium X-ray lenses down to around 10 μm. With further focussing using a mirror system that will be installed in 2026 the beam focus will be a few μm.

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Update on the European Spallation Source

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The European Spallation Source (ESS) in Lund is preparing for the delivery and use of its first neutrons. This year will mark important milestones in the project including the start of commissioning of the accelerator with beam on dump foreseen in March and the final delivery on site of some of the very first instruments.

In steady state operation the spallation source will provide the highest neutron brilliance, allowing for fast experiments on more and more complex systems. The unique long-pulse neutron source, will enable also better resolution and flexibility in experiments.

An update will be given on recent progress in the construction and preparation of future scientific activities. The process for organising the transition to an international user facility will be outlined as well as the challenges ahead.

An update on the recent initiatives towards the definition of future neutron instruments will be provided.

The European Spallation Source in Lund, Sweden

Structural and biochemical optimization of a urethane degrading amidase

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Global plastic production surpassed 400 million tons in 2022, underscoring the urgent need for better recycling strategies. While enzymatic PET hydrolysis is now industrially viable, efficient enzymes for other plastics like polyurethanes (PURs) remain scarce. Recently, amidase signature (AS) family enzymes capable of breaking urethane bonds in PUR analogs have been identified. Here, we report high-resolution crystal structures of the AS enzyme UMG-SP3 in three states: ligand-free, bound to a transition state-mimicking inhibitor, and bound to a PUR degradation product. These structures reveal a conserved core, a catalytic triad, and notable loop flexibility, with Arg209 in loop 3 showing two conformations upon ligand binding. Structure-guided studies identified key features enhancing urethane and amide bond hydrolysis. These insights advance our understanding of urethanase activity, supporting future PUR recycling efforts.

Seeding a phase transition with correlated disorder

Simon Wall
Aarhus University

Optical excitation of solids enables a rapid route to control material properties through non-equilibrium pathways. Due to the spatial coherence of the laser pulse and the short temporal duration, it was assumed that phase transitions were driven by coherent lattice motion - each unit cell responding in the same way and at the same time to the driving field.

However, the advent of X-ray lasers has enabled new methods to probe materials. Particularly, the ability to observe dynamics in the diffuse scattering have shown that light-induced phase transitions can be driven by spatially incoherent local structural changes and not the coherent pathway previously assumed, even on the ultrafast timescale.

In this talk, I will discuss how diffuse X-ray scattering can reveal that weak pulses of light can induce both long-range coherent and short-range incoherent distortions in the solid, and that the short-range fluctuations, or correlated disorder, that can be used to reduce the energy barrier associated with the light-induced phase transition, opening a new route for material control in the time domain.