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Scott C Dahl, *Carter Francis, Prof. Paul M Voyles*

112 Sub-surface Temperature Evolution Mapping during Laser Powder Bed Fusion via In-situ XRD
Junye Huang, *Andrew Chihpin Chuang, Jiandong Yuan, Minglei Qu, Qingyuan Li, Prof. Lianyi Chen*

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Wonhyuk Jo, *Changwan Ha, Jaeyong Shin, Ki-jeong Kim, Kyung-Tae Ko, Jehan Kim*

P114 X-ray photon correlation spectroscopy of vicinal oxide surfaces
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Tadesse Billo Reta, *Yan Li, Eric Dufresne, Hua Zhou, Supratik Guha, Dillon Fong*

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Robert Aymeric

Oral Presentation #1

Bridging the Timescales Between Coherent Diffractive Imaging and X-ray Photon Correlation Spectroscopy

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Understanding the behaviour and function of materials at the nanoscale necessitates the use of in situ and operando characterization approaches. Coherent X-ray analysis techniques, such as coherent diffraction imaging (CDI) and X-ray photon correlation spectroscopy (XPCS), are becoming quite well-suited for this purpose. CDI, and the scanning form

ptychography, are able to produce images with nanoscale spatial resolution information [1]. This, however, requires a high signal-to-noise ratio (SNR) in oversampled speckle patterns to enable convergence of the phase retrieval algorithms. XPCS, alternatively, correlates the speckle information in time and thereby is not bound to the same SNR requirements. This has allowed XPCS to be able to routinely be applied to the study of dynamic systems [2].
In this talk, I will discuss the underlying principles behind different coherent diffraction analysis techniques which can be used to characterize nanoscale systems. I will then show results from a proof-of-principle experiment we performed at the P10 beamline at PETRA III where XPCS and CDI were simultaneously combined to investigate the Brownian motion of gold nanoparticles [3]. These results demonstrate the complementary potential of combining both techniques, where XPCS provided accurate ensemble-averaged information on the diffusion characteristics, while the dynamics of individual nanoparticles as well as the process of agglomeration was observed by CDI.

Sub-microsecond XPCS from Fluctuation Dynamics in Liquids

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The combination of new pixel-array detectors that record photon arrival times [1] with the very high coherent X-ray flux from 4th generation synchrotron sources enables XPCS studies of dynamics in the nanosecond time range [2]. Here we present results from recent studies of fluctuation dynamics in liquids relevant to chemical separations, carried out at the European Synchrotron Radiation Facility and the Advanced Photon Source. These multicomponent liquids exhibit incipient phase separation, leading to large equilibrium composition fluctuations that produce small-angle X-ray scattering [3-5]. Understanding the dynamics of these fluctuations is a goal with both fundamental and practical implications. The detector is sufficiently fast to resolve the time structure arising from the fill pattern of the storage ring. The periodic fill pattern introduces strong oscillations into the measured time correlation function. We discuss methods to remove this structure from the measured time correlation, revealing the dynamics in the liquid. This allows us to test theoretical relationships between fluctuation dynamics, solution thermodynamics, and critical phenomena, providing overlap in time and length scales between experiments and molecular dynamics simulations.

Unraveling dual-timescale Epoxy Resin Cure Dynamics by Simultaneous XPCS–NMR Measurement

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Dynamics in materials encompass a vast range of spatial and temporal scales yet probing hierarchical behavior under nonequilibrium conditions remains a significant experimental challenge. X-ray photon correlation spectroscopy is well-suited for investigating dynamics at mesoscopic length scales, while time-domain nuclear magnetic resonance captures fast, localized molecular motions. Here, we introduce the first integrated XPCS–TD-NMR platform that enables simultaneous, real-time measurements across these disparate scales. We demonstrate its application to epoxy resin curing, directly correlating mesoscopic collective dynamics with microscopic molecular relaxation in a nonequilibrium system. TD-NMR resolved two distinct relaxation components from the earliest stages of curing, while XPCS revealed multiple dynamical regimes, including a slow, solid-like mode associated with gelation. The combined measurements show that different dynamical processes dominate at various curing stages and length scales, underscoring the intrinsic multiscale nature of epoxy network formation. This integrated approach provides a powerful tool for investigating dual-timescale polymer dynamics and offers new opportunities for rational optimization of curing processes and design of advanced functional materials.

In Situ and Operando Soft X-ray STXM and Ptychography at the ALS and ALS-U

Alexander S. Ditter[1], *David A. Shapiro*[1], *Young-Sang Yu*[2], *Chunjoong Kim*[2]
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In situ and operando measurements in soft x-ray (< 2 keV) scanning transmission x-ray microscopy (STXM) and ptychography offer valuable insight into nanoscale chemical changes in energy materials, but the low transmission of soft x-rays through materials make these experiments rare and challenging. Nonetheless, such experiments are becoming more common at Advanced Light Source Beamline 7.0.1.2 (COSMIC Imaging) where this problem is mitigated by leveraging in situ gas heating and liquid electrochemistry cells originally designed for use in tunneling electron microscopy (TEM) systems. Recent advancements of fast-scanning STXM and optimized ptychography have enabled higher time resolution of chemical mapping at the nanoscale. Here, we will show how this technology has enabled new areas of research including study of the phase change of LiFePO4 at high temperatures and the study of actinide chemistry in uranium oxides among other examples from battery and catalysis research [1-3]. These efforts will be discussed in the context of the increased coherent flux available at 4th generation light sources like the Advanced Light Source Upgrade (ALS-U) which is anticipated to drastically improve measurement times, leading to higher throughput and the availability of new science.

Hydrogen-Driven Dislocation Dynamics in Stainless Steel Probed Using In Situ Bragg Coherent X-ray Diffraction Imaging

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Hydrogen embrittlement (HE) remains a major obstacle to the safe deployment of hydrogen-based energy systems, degrading the structural integrity of metals used in production, storage, and transport infrastructure. Although simulations and thin-sample microscopies have proposed competing nanoscale mechanisms, direct three-dimensional measurements of hydrogen-induced dislocation behavior in bulk materials have remained inaccessible.

Here, we leverage in situ Bragg coherent X-ray diffraction imaging (BCDI) to achieve the first real-time, three-dimensional (3D) visualization of hydrogen-driven dislocation and strain field evolution inside an individual bulk grain of austenitic 316 stainless steel. BCDI uniquely enables non-destructive, phase-sensitive imaging of lattice displacement fields with nanoscale spatial resolution and high strain sensitivity, allowing us to resolve a 3D strain map associated with a single dislocation embedded deep within the material.

By continuously tracking an individual dislocation during hours of hydrogen charging, we directly quantify hydrogen-enhanced dislocation mobility and strain relaxation in the absence of applied stress. The phase-retrieved displacement fields reveal hydrogen-promoted unpinning and pinning events, as well as a measurable attenuation of the dislocation's elastic strain field—providing the first direct 3D experimental evidence of hydrogen elastic shielding in a bulk metallic system.

These results demonstrate the power of BCDI to capture dynamic defect physics under operando conditions and establish a new experimental framework for interrogating hydrogen–defect interactions in structural alloys. By providing quantitative nanoscale benchmarks under realistic conditions, this work bridges the gap between simulation and bulk behavior and can potentially advance predictive, multiscale modeling of HE. More broadly, it showcases BCDI as a transformative tool for understanding defect-mediated degradation mechanisms critical to the development of hydrogen-resistant materials for pipelines, storage systems, aviation, and nuclear energy infrastructure.

Oral Presentation #6

Validating hydrodynamic simulations of inertial fusion energy low density foams with x-ray ptychographic tomography and ultrafast x-ray phase contrast imaging

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The 2022 National Ignition Facility achievement in fusion ignition has spurred an international race to achieve practical fusion energy [1,2]. Since then, NIF has achieved scientific breakeven at least eight times meaning more fusion energy was released (up to 8.6 MJ) than was incident into a tritium-deuterium fuel capsule with 192 nanosecond lasers (~2 MJ). In 2024, the US Department of Energy - Fusion Energy Sciences program created three national Inertial Fusion Energy – Science and Technology Accelerated Research (IFE-STAR) Hubs. In the RISE Hub, we are seeking to develop aerogel and 3D printed foams for IFE fuel capsules. These foam fuel capsules may improve IFE implosion symmetry and control and thus increase IFE yield. However, characterization of static nanometer scale structure and dynamic ultrafast response of these foams is critical to validation of the hydrodynamic simulations and accurate prediction of IFE yield. Here we will report on our efforts to determine the nanometer scale structure and dopant level of the low-density foams via x-ray ptychographic tomography at the Advanced Photon Source and Linac Coherent Light Source (LCLS) [3,4,5]. Furthermore, we have studied the laser shock response at the Matter in Extreme Conditions Instrument at the LCLS with quantitative dynamic density retrieved from single shot x-ray phase contrast imaging and Talbot interferometry [6-9]. We have studied both low density aerogel and two photon polymerized 3D printed foams at densities around 25 mg/cm^3. We are currently seeking to constrain xRAGE and FLASH hydrodynamic models of these foams to improve the accuracy of the designed high-yield experiments for direct drive IFE. The accuracy of these models will be critical for developing IFE schemes with validated nanometer scale structure and dynamic response to improve accuracy of the fusion yield that will inform fusion pilot plant designs.

Capturing Single-Shot Videos with Coherent Lensless Imaging and Structured Illumination

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There are two main families of X-ray methods which exploit coherence: those based on X-ray photon correlation spectroscopy (XPCS), which study the dynamics of samples evolving over time, and those based on coherent diffractive imaging (CDI), which capture images of single moments in time. Increasingly, researchers are blending the two, using new analysis techniques to capture time-series of images [1] and studying the relevant dynamics directly in real space. It is natural to consider implementing such ideas at a free electron laser (FEL), where time-resolved microscopy experiments are popular to study, for example, magnetic dynamics in thin films [2]. However, these experiments are limited to pump-probe studies of repeatable samples, for a simple reason: the existing methods capture one image per FEL pulse.

In this work, we report on the development of a coherent lensless imaging method which can capture single-shot videos, rather than single-shot images, with the goal of circumventing this limitation. To enable this, we developed a unique geometry which uses a diffractive optic both as a split-and-delay system and to imprint a structured illumination pattern into the light, allowing for each frame of data to be recovered using randomized probe imaging [3].

To demonstrate the method, we present the results of an experiment in which one shot of the FERMI FEL [4] captured an eight-frame video of a single ultrafast demagnetization event occurring in a thin GdCo film over a 500 femtosecond time window. We highlight the relevant experimental and algorithmic considerations, show the key experimental results, and discuss the implications for future experiments and the design of future FEL light sources.

Submicron-resolution propagation-based phase-contrast imaging at 100 keV

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High-energy X-rays have strong penetration power, making them particularly useful for imaging strongly absorbing objects such as metallic components, devices enclosed in metallic housings, and samples in high-pressure environments. For example, the absorption length of copper increases from ~5 μm at 10 keV to ~2 mm at 100 keV, an increase of more than two orders of magnitude. However, the absorption contrast decreases significantly at such high X-ray energies, limiting sensitivity to fine structures and small density variations.

Here we demonstrate submicron-resolution imaging at 100 keV using propagation-based phase-contrast imaging in a Gabor-type in-line holographic configuration. Phase contrast provides sensitivity two to three orders of magnitude higher than absorption contrast, facilitating the visualization of fine structures. By using divergent illumination from a nanofocused beam generated by graded multilayer Kirkpatrick–Baez (KB) mirrors, submicron spatial resolution was achieved.

Experiments were performed at the BL05XU beamline of SPring-8. The beamline provides a high-flux 100 keV pink beam with a bandwidth of ~1% by combining a short-period in-vacuum undulator (IVU-II) with a double-multilayer monochromator (DMM). The beam was focused to a spot of 0.3 × 0.4 μm using graded multilayer KB mirrors, providing a photon flux of ~3×10^11 photons/s at the sample position. The transmitted intensity patterns were recorded using a scintillator-lens-coupled detector. Phase images were reconstructed from the recorded intensity patterns using phase-retrieval algorithms. The spatial resolution was evaluated using a 0.5-μm-thick gold test chart, resolving a half-pitch of 250 nm. Tomographic imaging of a 3-mm-thick laser-welded copper sample revealed cavity defects smaller than 5 μm. These results demonstrate that high-energy propagation-based phase-contrast imaging is a promising method for imaging strongly absorbing objects, such as thick metallic components, with nanoscale spatial resolution.

Coherence and Structural Information in Intense X-ray–Driven Systems: From Scattering to Fluorescence Correlations

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Coherent X-ray imaging with intense X-ray free-electron laser (XFEL) pulses operates in a regime where ultrafast electronic dynamics, rather than static structure, can govern the coherence and information content of measured signals. Rapid ionization and electronic relaxation during the pulse create transient nonequilibrium states [1] that modify both scattering and emission processes. Understanding how these dynamics influence coherence is therefore essential for interpreting XFEL imaging experiments.

In this presentation, I discuss two complementary manifestations of coherence in strong-field XFEL interactions. First, transient electronic resonances that emerge during ultrafast ionization dynamics can strongly modify resonant X-ray scattering pathways [2-6]. These transient states enable interference between elastic scattering and resonance fluorescence channels, revealing how electronic dynamics shape the coherence properties of scattered X-rays.

Second, I examine fluorescence intensity correlation [7], sometimes referred to as incoherent diffractive imaging [8], which extracts structural information from second-order correlations of X-ray fluorescence, closely related to Hanbury Brown–Twiss intensity interferometry. Even when conventional scattering signals are degraded by radiation-induced ionization and the presence of delocalized electrons, fluorescence correlations can encode structural and elemental information and may provide an alternate route to imaging under intense XFEL conditions.

These results highlight how ultrafast electronic dynamics shape both scattering and fluorescence coherence in XFEL experiments and suggest new opportunities for exploiting emission-based correlations alongside conventional scattering for imaging structures and dynamics of nanoscale systems.

Nanosecond resolving capability of the CITIUS detector enabled by “spectral streaking”

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In this talk, I will present a novel spectral streaking mode of the CITIUS detector, a latest-generation high-repetition-rate detector developed by RIKEN SPring-8 Center in collaboration with Sony (1,2). By leveraging its low-noise pixel readout and fast shutter response, we demonstrate nanosecond-resolving capability. In particular, the detector resolves scattering from two x-ray free-electron laser (XFEL) pulses separated by only 70 ns, generated in the nanosecond two-bunch mode at the Linac Coherent Light Source (3).

Using a static scattering target, we show that the spatial intensity correlation of coherent scattering pattern pairs can sensitively detect subtle trajectory mismatches between the nanosecond pulse pairs, demonstrating the detector’s utility as a diagnostic for optimizing two-bunch orbit control in the ongoing cavity-based XFEL project (4).

This nanosecond time range also opens new opportunities for ultrafast x-ray photon correlation spectroscopy (XPCS), enabling studies of dynamic processes relevant to materials growth, stability, and function, as well as fundamental phenomena such as the glass transition, liquid–liquid phase transitions, and water anomalies. I will also present an analysis strategy, validated by simulation, for using this mode to perform XPCS measurements of nanosecond dynamics.

Ultrafast Coherent Diffraction Imaging and Bragg CDI on individual Gold Nanoparticles

Rasmus Buchin[1,6], *Robert G. Radloff*[1,6], *Jan Leutloff*[1,2,6], *Nils Muthreich*[2], *Sarah Grimm*[2], *Ichiro Inoue*[3], *Slawomir Skruszewicz*[1,6], *Hankai Zhang*[5], *Sven Gieschen*[1,6], *Holger Meyer*[1,6], *Simon Dold*[4], *Xin Liu*[4], *Raphael de Wijn*[4], *Lena Worbs*[4], *Fabian Trost*[4], *Yonhee Kim*[4], *Konstantin Kharitonov*[4], *Johan Bielecki*[4], *Christoph Bostedt*[5], *Florian Schulz*[1], *Stephan Kuschel*[2], *Tais Gorkhover*[1,6]
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Ultrafast and intense X-ray free electron laser (XFEL) pulses can visualize non-equilibrium dynamics on the femtosecond time scale with high spatial resolution at single nanoparticle (NP) level . Single exposure coherent diffraction imaging (CDI) of individual nanospecimen has been so far limited to a few nanometers. The limiting factor is sample bleaching through photo-ionization and resulting low photon signal in higher scattering angles.

Our preliminary data analysis from experiments at LCLS and the EuXFEL indicates, that transient resonances might overcome bleaching in images recorded with intense, hard X-rays pulses and increase the spatial resolution. We have recorded small and wide-angle scattering (Bragg CDI) from Au NPs with sizes ranging from 4-70 nm. We observe multiple Bragg peaks from a single domain 10 nm NP, which exhibit multiple higher diffraction orders. Thus, a reconstruction of the NP's shape from multiple orientations is possible from a single image. The small angle X-ray diffraction signal reaches up to 1 nm resolution in images of samples, where the best previously reported reconstruction achieves only 2 nm resolution. Our data also suggests that 10 fs FEL pulses might be too long to observe true atomic resolution in single metal particle imaging.

By combining small angle CDI and wide angle BCDI, we obtain complementary structural information, with both techniques capturing multiple diffraction orders. This proof-of-concept study highlights a pathway for improving single-shot resolution and offers new insights into ultrafast structural dynamics at the nanoscale.

Coherent extreme-UV imaging of ultrafast phenomena at the nanoscale

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Enabling lensless imaging of complex structures with nanometer resolution, coherent extreme ultraviolet and X-ray sources have transformed nanoscale microscopy [1-3]. New challenges emerge when extending these approaches to ultrafast phenomena in solids, where many technologically relevant processes occur on femtosecond timescales and often produce only weak scattering signatures. In such systems the relevant signal can be orders of magnitude weaker than the absorption contrast from strongly scattering nanostructures, making the detection of subtle transient changes particularly demanding. Applying coherent imaging to such weak-signal dynamics requires balancing spatial and temporal resolution while maintaining strict control over reconstruction fidelity. A central challenge is distinguishing genuine material dynamics from reconstruction artifacts and other source-dependent effects that vary between different coherent light sources.

Here we present an ultrafast coherent extreme-UV imaging platform based on high-harmonic generation (HHG). Imaging magnetic spin textures during ultrafast demagnetization as a benchmark, we achieve sub-wavelength spatial and femtosecond temporal resolution [4]. Owing to full polarization control of the setup, the measurements provide element-specific and spin-sensitive contrast in various first-row magnetic metals. Furthermore, we demonstrate sub-nanometer precision in tracking nanoscale magnetic spin textures, providing the first direct real-space insight into ultrafast domain-wall dynamics during femtosecond demagnetization and the role of non-local spin transport – two central and long-debated topics in ultrafast magnetism.

Our instrumentation provides a table-top testbed for developing and validating reconstruction strategies in the weak-signal regime. In addition, we have tested our coherent imaging approach at synchrotron and free-electron-laser facilities, enabling direct comparison across different coherent probe types and revealing both shared and source-specific methodological challenges.

Nanoscale collective excitations: EUV Transient Grating

Laura Foglia

The properties and functionalities of solids, molecules and hybrid compounds used in modern technology is dictated by the interplay between the electronic, lattice and spin degrees of freedoms.

Pump-probe techniques are ideal to selectively investigate their time evolution and disentangle complex processes. Their extension to the Extreme Ultraviolet and X-ray regime allows element specificity and the possibility to access meso- and nanoscopic length scales. In this talk I will present an alternative approach, developed at the FERMI free electron laser (FEL), where the sensitivity to the sub-100 nm length-scale is obtained exploiting extreme ultraviolet transient gratings (EUV TGs). First, I will briefly address the applications of EUV TG to the investigation of the thermoelastic properties of materials on a previously inaccessible wavelength range. Then, I will discuss the potential of EUV TGs in other contexts, beyond its original goal. Building upon the first demonstration of magnetization TGs, I will discuss the newest demonstrations of transient magnetization dynamics at the nanoscale.

To conclude, I will review further approaches exploiting the nanoscale periodically structured photoexcitation besides TG spectroscopy.

Measuring nanosecond fluctuations in magnetic spin textures by counting photons

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When a magnetic spin texture undergoes a phase transition, instabilities between the two competing phases often result in spatiotemporal fluctuations that diverge at the phase boundary. Measuring dynamics close to these phase boundaries is especially challenging since the experimentally observable signal that results from the order in the system is heavily reduced. To overcome this low signal challenge, x-ray photon fluctuation spectroscopy (XPFS) is a technique that counts individual photons to quantify the qualitity of the speckle scattering pattern, i.e. the speckle contrast. By mapping the distribution of signal per speckle count rates to this contrast, and comparing single x-ray pulses with pairs separated by a predetermined delay time, we can access dynamics intrinsic to the magnetic spin textures. Here I present new results from a FeGd skyrmion lattice system near the stripe ordering boundary, as well as describe nanosecond fluctuations at a phase boundary between different spin textures in amorphous FeGe. These recent developments of uncovering nanosecond dynamics where measured at the ChemRIXS endstation at the Linac Coherent Light Source.

Femtosecond Coherent X-ray Nanodiffraction Imaging of Stochastic and Defect-Mediated Structural Phase Transition in FeRh

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First-order phase transitions, characterized by discontinuities in the order parameter, proceed via nucleation and growth under equilibrium conditions. However, on ultrafast timescales, before thermal equilibrium is established, the underlying nonequilibrium and nanoscale structural dynamics remain poorly understood. Here, we employ a newly developed nanofocusing capability at the Linac Coherent Light Source free-electron laser to investigate the spatiotemporal dynamics of the laser-induced antiferromagnetic-to-ferromagnetic (AFM–FM) phase transition in a FeRh thin film grown on MgO, which is accompanied by an ultrafast lattice expansion. Spatial inhomogeneity of the transition is examined through two complementary approaches: scanning X-ray nanodiffraction imaging to probe sub-micrometer-scale structural dynamics, and time-dependent speckle patterns arising from coherent X-ray diffraction to assess nanometer-scale structural dynamics. These measurements reveal ultrafast stochastic nucleation of the FM phase within a few picoseconds, generating a transient strain inhomogeneity. Local defective regions, such as those associated with non-uniform film growth, exhibit markedly distinct nucleation and growth dynamics. The nanoscopic insights into ultrafast structural dynamics provided by femtosecond coherent X-ray nanodiffraction imaging have important implications for optimizing heat-assisted magnetic recording at the nanoscale.

The coherent diffractive imaging beamline at National Synchrotron Light Source II

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Coherent diffractive imaging continues to produce unique insights into the structure and dynamics of materials at nanoscale resolution. At National Synchrotron Light Source II(NSLS_II)—following first light in December 2025—a new beamline designed to provide novel controlled x-ray illumination, sample environments, and experimental geometries is being commissioned and will soon be ready for user science. The design considerations, beamline optical system simulations, endstation provisions, and early performance will be discussed.

The CDI beamline's source is provided by an 18-mm-period in-vacuum undulator and the 3 GeV electrons from NSLS-II. The undulator has a variable taper feature, delivering an increased x-ray bandwidth of at least 5% RMS at 10 keV. The optical system is comprised of two bendable x-ray mirrors in conjunction with two fixed-figure mirrors to provide a sample illumination that allows variable coherence properties in a "zoomable" x-ray focal spot of about 1 to 10 microns in lateral size. Thus, the optical design provides a unique opportunity to tailor beam properties to the needs of any particular coherent imaging experiment. The final optic provides a very long working distance of approx. 1.5 m and the sample-to-detector distance can be varied from 0.5 m to 10 m. The long sample-to-detector distance and the detectors' pixel pitch are selected to allow nanoscale-resolution spatial mapping of micron-sized objects without scanning the sample's position in the beam, although provisions for scanning do exist. Two area detectors will be independently positionable, allowing for simultaneous measurements in either or both of the forward-scattering and a Bragg-reflection geometry. The angular coverage of the detector system varies from approx. 70(V) x 120(H) to 11(V) x 120(H) degrees as a function of sample-to-detector distance.

The CDI beamline presents an exciting capability for routine, high-stability coherent imaging measurements and a uniquely-capable test-bed for the development and refinement of future imaging methods. CDI is on track to complete its technical commissioning this year and accept general users in 2027.

Pushing compute onto detector silicon

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Modern X-ray detectors now generate data streams so large that data movement increasingly limits scientific discovery. We present a paradigm that pushes key data-reduction algorithms directly onto or near detector silicon.

We report on the SparkPix-RT2 detector, a charge-integrating pixel detector co-developed by Argonne National Laboratory (ANL) and SLAC National Accelerator Laboratory, integrating on-chip compression (user-selectable lossless and lossy modes) at continuous frame rates up to 100 kHz. Beamline tests of SparkPix-RT2 equipped with a CdTe sensor will be presented. Rather than transmitting every pixel of every frame, the detector produces a compact representation in real time, reducing data rates while preserving scientifically relevant features.

Building on this foundation, we are developing SparkPix-matmul, a next-generation ASIC architecture that implements matrix–multiply operations directly in detector logic. This enables principal-component and related projections at the detector edge. Using this architecture, we have demonstrated that homomorphic compression permits direct computation of two-time correlation functions for X-ray photon correlation spectroscopy (XPCS) without decompression, establishing a pathway toward on-chip XPCS analysis. Beyond compression, the approach supports additional near-detector reduction, including radial integration. Programmable on-chip weight matrices allow experiment-specific optimization, effectively “training” the detector for a given measurement.

Detector ASICs, however, are silicon-area constrained to the periphery of the pixel matrix. As data rates scale toward terabits per second, more sophisticated processing must migrate to nearby scientific chipsets fabricated in advanced CMOS nodes and connected through high-speed interposer-based integration. In this heterogeneous model, X-ray detectors begin to resemble modern processing units, with sensing and computing co-designed and co-packaged to overcome interconnect bottlenecks and enable adaptive, high-throughput experiments at next-generation light sources.

Advanced KB focusing mirrors for coherent X-ray imaging without secondary source aperture

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The multi-bend achromat upgrade of the storage ring lattice significantly reduces the X-ray source size and divergence, particularly in the horizontal direction. At SPring-8-II, the upgrade of the SPring-8 facility [1], the number of spatially coherent modes [2] at 8 keV in the horizontal direction is expected to decrease from the current value of 110 to approximately 3.6. Under such conditions, the use of a secondary source aperture is no longer required, and the focused beam obtained by direct demagnification of the source can be utilized for coherent X-ray imaging.

To exploit this capability, we have developed advanced Kirkpatrick–Baez (AKB) mirrors [3] for direct focusing of fourth-generation synchrotron radiation sources. The AKB optics employ mirror configurations based on Wolter geometry, which suppress coma aberration and enable stable and efficient nanofocusing.

For coherent imaging techniques such as X-ray ptychography, maximizing coherent flux is essential, while maintaining a stable illumination wavefield is equally important. The coma-suppressing characteristics of the AKB optics are advantageous for providing highly stable illumination. The newly developed AKB mirrors are designed to produce a focal spot of 200 × 300 nm² with an angular tolerance of 200–500 μrad, delivering a photon flux of 10^{11}-10^{12} photons/s/0.01% bandwidth. For tightly focused nanoprobes, particularly for applications such as holotomography, achieving a large demagnification factor within the limited beamline length is crucial. We have therefore developed a nanofocusing system based on AKB mirrors with Wolter type III geometry [4], targeting a focusing spot size of 7 nm with photon flux of 10^{13} photons/s/1% bandwidth.

This presentation will describe the mirror designs, fabrication/commissioning progress, and the achieved focusing performances.

Probing crystal structure and defect-driven reactivity using Bragg Coherent Diffraction Imaging

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The use and improvement of state-of-the-art coherent X-ray imaging capabilities that leverage the unique characteristics of fourth-generation hard X-ray sources, such as the Advanced Photon Source Upgrade (APS-U), are essential to progresses in multiple scientific areas in chemistry and materials science. These techniques enable direct observation of the spatial distribution of defects at surfaces and within three-dimensional nanocrystals, providing a route to establishing robust structure–property relationships that govern interfacial reactivity.

In this talk, I will present two recent studies in which we used Bragg coherent diffraction imaging (BCDI) to determine the three-dimensional (3D) electron density and atomic displacement field of calcite ($CaCO_3$) crystals. In the first study (1), BCDI reveals the internal structure of calcite crystals synthesized via two distinct routes. The reconstructions show striking differences in crystalline structure: one method yields true single crystals, whereas the other produces multidomain particles, consistent with a nonclassical crystallization pathway involving oriented attachment of smaller nanoparticles. In the second study (2), we exploit BCDI to quantify changes in strain and morphology of individual calcite crystals before and after dissolution in a Pb-containing aqueous solution at pH 3.7. The reconstructions indicate that dissolution proceeds preferentially at tensile-strained regions near macrosteps. These results demonstrate that the local reactivity of calcite—quantified as the spatial distribution of dissolution rates—is strongly correlated with pre-existing strain in as-grown calcite nanocrystals.

Imaging Calcite Surface Topography using Coherent X-ray Reflectivity

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Our understanding of how interfacial topography and defects influence interfacial reactivity remains incomplete due to the difficulty of imaging buried interfacial topography (e.g., in complex operando environments) and imaging at sub-nm-scales. The increasing availability of coherent X-ray beams at fourth-generation synchrotron facilities is enabling new imaging approaches. In this work, we demonstrate the feasibility of imaging the surface topography of calcite ($CaCO_3$), in three-dimensions, using coherent X-ray reflectivity (CXR). This method utilizes the coherent X-ray reflectivity signal—the crystal truncation rod (CTR)—measured during a rocking scan to reconstruct interfacial topography. The approach builds on the principles of Bragg Coherent Diffraction Imaging (BCDI), which reconstructs particle morphology and strain from 3D reciprocal-space maps of a Bragg peak, and extends them to the imaging of interfaces through the surface truncation rod. We show that the 3D coherent reflected intensities along the CTR can be successfully phased using conventional phase-retrieval algorithms to produce a complex interfacial density whose phase directly encodes surface topography. Although the resulting images have a vertical resolution of ~30 nm, the phase of the interfacial density provides sub-nanometer sensitivity to the surface height—representing a ~100-fold improvement beyond the nominal resolution limit. The resulting interfacial images reveal terraced surface topographies having height variations that range from ~300 nm to nearly atomically flat across the beam footprint, for free surfaces and buried interfaces of a micron-scale calcite crystal, as well as for the free surface of an extended macro-crystal.

In Operando Bragg Coherent Diffraction Imaging of Functional Materials in Complex Experimental Environments

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As devices trend deeper into the nanoscale, high-resolution characterization techniques become essential for optimizing design. Observing functional materials is challenging, especially in complex or novel operating conditions. Characterization techniques must therefore be non-destructive, and robust enough to provide high-quality data in realistic operating environments. Here, we demonstrate that Bragg Coherent Diffraction Imaging (BCDI) can be effectively utilized to interrogate functional materials in operando at high resolution.

We report three-dimensional imaging of defects, crystal morphology, and strain dynamics in individual Bi2WO6 (BWO) nanoflakes using (BCDI) under operando temperature, gas, and light-driven conditions. We observe that Argon (Ar) gas flow stabilizes the reaction environment, while a mixed Hydrogen--Nitrogen (H2 + N2) flow induces a hydrogen-triggered semiconducting-to-metallic (SM) electronic phase transition accompanied by a structural transformation, as supported by density functional theory (DFT) calculations. Both DFT and BCDI analyses reveal that during the SM phase transition, a new structural phase nucleates near defects and propagates inhomogeneously. Notably, we observe the onset of nanoscale cracking, driven by localized strain accumulation and environmental cycling, which increases surface area and potentially introduces new reactive sites.

We also show the strengths of BCDI in characterizing the restructuring of ferroelectric domains in response to the stimulus of a Twisted optical beam. We present experimental evidence demonstrating that dynamic control of novel domain states is achievable in the quasi-2D ferroelectric CsBiNb2O7 using a continuum of twisted ultraviolet (UV) light, which resonantly excites the zone-center ferroelectric mode and the zone-boundary octahedral tilting mode. We develop and utilize in-situ BCDI, Raman spectroscopy, and DFT calculations to detect and three-dimensionally resolve the resultant ionic displacement field and changes in ferroelectric polarization texture. This approach allows us to directly observe deterministic and reversible twisted light-induced strain and ionic displacements within the unit cell, leading to significant microscopic changes in ferroelectric polarization.

Structural Heterogeneity and Dynamics of Disordered Materials Determined by Machine Learning Enabled 4-Dimensional Scanning Transmission Electron

Jinwoo Hwang

This presentation will showcase recent advances in 4-dimensional scanning transmission electron microscopy (4D-STEM) to determine the detailed medium range ordering (MRO) that constitutes nanoscale structural heterogeneity governing important properties of a wide range of disordered materials, including metallic glasses, amorphous oxide films, amorphous chalcogenides, and polymer glasses. Using an electron probe with a size of about 1–2 nanometers, 4D-STEM acquires nanodiVraction patterns from a large sample area, providing details on the type, size, and distribution of MRO, as well as the dynamics of atomic rearrangement under electron dose. 4D-STEM generates a large number of nanodiVraction patterns for analysis, which inherently makes it a big data problem. Our recent eVorts demonstrate the application of a machine learning algorithm based on a convolution transformer neural network to 4D-STEM nanodiVraction patterns, revealing unprecedented details of MRO structures across various compositions in Zr-based metallic glasses and providing important insights into how properties such as yield strength and plasticity limit change even with small variations in composition. We also compare nanoscale structural heterogeneity information obtained from 4D-STEM with pair distribution functions acquired using synchrotron X-ray diVraction to understand how these two measurements correlate and to resolve discrepancies in how MRO is defined based on key features in their respective data. The presentation will also discuss recent results from amorphous oxide and chalcogenide films to understand how MRO aVects crystallization behavior, as well as the evolution of nanoscale molecular ordering domains in semiconducting polymers.

Direct Observation of Facilitated Dynamics in a Supercooled Liquid via Electron Correlation Microscopy

Po-cheng Kung[1], *Scott Dahl[1], Ajay Annamareddy[1], Angan Mukherjee[1], Victor Zavala[1], Dane Morgan[1], Paul Voyles[1]*
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As temperatures approach the glass transition temperature Tg, supercooled liquids (SCLs) often exhibit heterogeneous dynamics characterized by local relaxation times that vary significantly across nanometer scales. Dynamic facilitation is a theoretical framework proposed to explain the underlying physics of this heterogeneity, suggesting that rare mobile domains formed during the early stage of the relaxation process can facilitate the relaxation of neighboring regions. Although this phenomenon has been observed in simulations [1], direct experimental evidence remains elusive.

To provide direct experimental evidence of facilitated dynamics in SCLs, we utilized electron correlation microscopy (ECM) via time-resolved four-dimensional scanning transmission electron microscopy (4D STEM). We developed a modified two-time correlation function—tailored for the large speckles and small real-space sampling volumes inherent to electron nanodiffraction—that probes local dynamics with high spatial and temporal resolutions. This approach allows for the direct observation of individual mobile domains and their inter-domain interactions, thereby capturing the mechanisms of dynamic facilitation.

Observations of Pd77.7Cu6Si16.3 SCL droplets revealed evidence of facilitated dynamics. By tracking domain decorrelation over twice the average structural relaxation time, we found that relaxation initiates at the surface, where the dynamics are accelerated. This relaxation then propagates inward, with slow central domains being progressively replaced via domain boundary propagation. We observed similar behavior in simulated nanodiffraction data from molecular dynamics trajectories of liquids. This pattern is consistent with the facilitated dynamics behaviors observed in simulations [1]. Analysis of the topology of decorrelated domains using the Euler characteristic demonstrates that droplets at lower temperatures exhibit higher degrees of dynamic facilitation. This result indicates a distinct shift in dynamic facilitation behavior as the temperature approaches Tg.

Nanofocused Microsecond XPCS Enables Spatiotemporal Mapping of Nanoparticle Diffusivity During Mesocrystal Assembly

Klara Suchan[1,2], *Matheus Gomes Ferreira*[1], *Leonardo Oliviero*[1,2], *Iason Andronis*[3], *Maik Kahnt*[2], *Foivos Perakis*[3], *Dmitry Baranov*[1], *Jesper Wallentin*[1]
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Nanoparticles (NPs) can self-assemble into highly ordered mesocrystals, in which long-range interparticle correlations give rise to collective phenomena. The degree of ordering critically determines the extent of these collective effects. NP diffusivity is hereby decisive for whether ordered assembly or kinetic arrest occurs but has remained challenging to access due to the microsecond timescales involved.

We address this with in situ X-ray photon correlation spectroscopy (XPCS) combining three recent advances: a fourth-generation synchrotron (MAX IV) providing ~100× higher coherent flux than third-generation sources, a nanofocused beam (70 nm) enabling spatially resolved measurements and enhanced contrast, and a prototype detector operating at 120 kHz frame rate giving access to microsecond dynamics. Together, these enable direct, spatiotemporally resolved quantification of NP diffusivity simultaneously with the evolving SAXS signal and local volume fraction throughout evaporation.

Applying this to 8nm $CsPbBr_3$ NPs, we observe a 30-fold slowdown of collective dynamics from 3 μs to 80 μs at volume fractions ~8%, far below geometric close-packing, driven primarily by hydrodynamic suppression rather than thermodynamic clustering. Spatial mapping reveals that regions up to 100 μm below the evaporation front maintain sufficient diffusive mobility for ordered mesocrystal formation, while regions further down undergo premature agglomeration and kinetic arrest. Our results establish hydrodynamic interactions as the decisive factor governing pathway selection in evaporative self-assembly and provide direct design criteria for improving mesocrystal yield through tailored solvent and ligand choice. More broadly, they demonstrate nanofocused XPCS as a powerful probe of spatially resolved NP dynamics in complex, evolving colloidal environments

From point defects to embedded nanoparticles, providing new insights into quantum materials with electron ptychography

James Lebeau[1]
[1]MIT

Multislice electron ptychography (MEP) is quickly becoming a powerful technique for three-dimensional, atomic-resolution analysis of point defects and implantation damage in quantum materials. In this presentation, we evaluate and demonstrate its quantitative capabilities across two proposed qubit hosts: SiC and CeO_2. For SiC, we will analyze depth-resolved MEP reconstructions of approximately 2000 nm³ volumes along the implantation direction, comparing them with pristine material to directly assess implantation-induced disorder. The reconstructed structure shows lattice damage reaching depths of about 100 nm, far beyond the range predicted by traditional implantation simulations that ignore crystallographic channeling. Multislice simulations show that this static disorder limits the visibility of both Er dopants and silicon vacancies in the damaged area. Beyond this zone, isolated silicon vacancies become identifiable, can be localized within a single unit cell along the beam direction, and used to analyze their local strain fields. Systematic simulations covering vacancy, antisite, and substitutional transition-metal dopants (V–W) on the Si sublattice, as well as variations in electron energy, dose, defocus, and convergence semi-angle, map the practical limits for detecting point defects in 4H-SiC. We will also demonstrate MEP's ability to quantitatively analyze nanostructured systems, such as SiC embedded within Si. Regarding Zr-doped CeO_2, we observe an increasing concentration of Zr interstitials leading to oxygen vacancies. To reliably identify chemical compositions despite challenges such as thermal vibrations, local distortions, reconstruction settings, and sampling, we extract multiple features from reconstructed depth profiles and classify them with a trained machine learning model trained on multislice-simulated MEP data. This method provides high-confidence identification of interstitial sites. Collectively, these studies establish multislice electron ptychography as a truly quantitative three-dimensional tool for examining defect chemistry, strain, and implantation-induced disorder. It opens a pathway to directly observe how processing and doping modify quantum materials at the atomic level.

Nanoscale Ptychography with a Broadband EUV and Soft X-Ray High Harmonic Source

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The extreme ultraviolet (EUV) and soft X-ray (SXR) spectral ranges are uniquely suited for metrology applications in microbiology, materials science, and non-destructive semiconductor inspection due to spanning the absorption edges of several relevant elements, e.g. silicon, carbon, and oxygen. Moreover, the long attenuation lengths of short wavelength light enables imaging of samples with micrometer-scale thickness. Advances in ultrafast laser technology have enabled the production of ultra-stable and spatially coherent EUV and SXR sources via high harmonic generation (HHG). The spatial coherence of these sources allows for the dissemination of coherent diffraction imaging (CDI) modalities, such as ptychography, into laboratories outside of large-scale facilities. However, if the driving laser is either in the mid-IR region or has a few-cycle pulse duration, the generated high-harmonic radiation is intrinsically broadband, which conflicts with the temporal coherence requirements of CDI. Multilayer mirrors can monochromatize the light at the expense of considerably lower integrated photon flux. By achieving a sub-micrometer spot-size at the sample, and utilizing reconstruction algorithms that account for dispersion of the probe and farfield propagation, we are able to relax the temporal coherence requirements of ptychography. Here, we report on sub-50 nm resolution ptychographic imaging using a 13.5 nm high harmonic source with up to 10% relative bandwidth, the largest spectrum used for an EUV ptychography experiment to-date. This increased the usable photon flux by a factor of three, compared to previous measurements at 3% relative bandwidth. Accommodating broad spectra will be critical for extending this methodology into the SXR regime, where state-of-the-art HHG sources show low brightness, demanding long measurement times. Moreover, for samples with significantly wavelength-dependent transmission and phase contrast, broadband illumination shows potential for spectroscopic imaging at the nanoscale.

Optimizing the Near-Field Ptychography acquisitions

William Chèvremont[1], *Peter Cloetens*[1]
[1]ESRF

Ptychography has emerged over the past 20 years for high resolution X-ray imaging. This is a coherent and lensless imaging technique which consists in acquiring images of the sample with lateral diversity. Considering the probe constant, it is then possible to retrieve the probe and the object in both phase and amplitude. The acquisition may be done in two different regimes. In the far-field one, a diffraction pattern is collected (Fraunhofer regime) and the sample is scanned with the probe, having some overlaps for each image. In the near-field one, a full-field image is collected at finite propagation distance (Fresnel regime) and most of the collected images overlap. This entails the advantage of faster full-field acquisition where only a small number of images are enough to cover a wide area. In order to reduce the total dose on the sample and the acquisition time required by near-field ptychography, some optimizations have been recently developed at the nano-imaging beamline ID16A of the ESRF. First, the control system of the nanopositioning stage has been upgraded with a fast real-time system, which allows better stability and less dead time for stabilization after displacement. Then, all the acquisition parameters have been fine tuned in order to accelerate the acquisition without compromises on the final reconstruction quality. This includes parameters such as exposure time and stabilization time as well as finding the best displacement pattern in order to reduce the required number of images for each projection. Finally, the tomographic acquisition is subdivided into subtomos allowing to track sample drift and eventually homogeneous sample deformation over time to be taken into account during the reconstruction process.

Coherent X-ray Methods to Track Nanoparticles from Biological Media to Intracellular Fate

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Coherent X-ray methods provide unique opportunities to investigate nanoparticle behavior in complex biological environments across multiple length and time scales. In this work, we present a correlative approach combining X-ray photon correlation spectroscopy (XPCS) and X-ray ptychography to investigate nanoparticle dynamics from biological media to intracellular organization in macrophages. XPCS measurements in complex protein-rich environments demonstrate that coherent scattering can distinguish protein corona formation from nanoparticle aggregation and quantify nanoparticle diffusion in situ, without dilution, fractionation, or optical labeling. These measurements provide direct access to nanoparticle dynamics in crowded biological environments that are not accessible by conventional light-scattering techniques. Building on these results, correlative cryogenic soft X-ray tomography and X-ray ptychography were used to investigate how nanoparticle distribution evolves inside cells as a function of dose and cell division. Three-dimensional imaging across multiple cell generations reveals that nanoparticle organization is not static but evolves systematically over time, with progressive perinuclear accumulation, changes in vesicular organization, and division-dependent redistribution and inheritance patterns. The results indicate that cell division plays a central role in the intracellular fate of nanoparticles, leading to non-trivial partitioning and long-term intracellular reorganization across successive generations. Together, these results demonstrate how coherent synchrotron X-ray methods enable multiscale studies of nanoparticle behavior, bridging colloidal dynamics in complex biological media with intracellular organization and long-term nanoparticle fate inside cells. This correlative approach illustrates the potential of coherent X-ray methods to connect nanoscale dynamics, cellular structure, and biological function within a single experimental framework.

Transport-Coefficient Approach to Resolving Nonequilibrium Dynamics in Colloidal Suspensions

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Multi-Bend Achromat (MBA) lattice upgrades at synchrotrons have greatly increased coherent X-ray flux, enabling X-ray Photon Correlation Spectroscopy (XPCS) to probe microscopic dynamics over previously inaccessible time and length scales. This opens the opportunity to study and resolve complex, non-equilibrium dynamics and transient phenomena in soft matter. However, full exploitation of these capabilities of upgraded synchrotrons for these studies is limited by current analysis frameworks that average out transient and non-equilibrium information.

We developed a transport coefficient approach that formulates XPCS dynamics in a Markov-chain framework including both internal interactions and externally imposed forces [1]. This yields a universal transport coefficient, J(t), that quantitatively characterizes time-dependent microscopic transport and can be extended to describe complex, non-equilibrium dynamical signatures. Validation using experimental and simulated non-equilibrium systems shows that the extracted J(t) and associated parameters recover known behaviors while providing enhanced sensitivity to heterogeneous and time-evolving dynamics.

We then applied this framework to study transient rheological phenomenon: the yielding of colloidal suspensions under deformation [2]. Using Rheology–XPCS combined with fast lubrication molecular dynamics simulations, we resolved the evolution of particle-scale dynamics and structure during yielding. Repulsive suspensions yield smoothly and uniformly, displaying Andrade-like deformation with minimal structural reorganization. In contrast, attractive suspensions exhibit delayed yielding and pronounced dynamical heterogeneity, consistent with shear banding. The transition is governed by transient dynamics at shear-band interfaces, where interfacial instabilities strongly influence the macroscopic rheological response.

Overall, the transport coefficient provides a compact, time-resolved descriptor that links XPCS observables to microscopic transport under non-equilibrium driving. As such, it offers a broadly applicable analysis tool for studying diverse dynamical phenomena with XPCS—beyond yielding—including start-up flows, stress relaxations, aging and rejuvenation, and other spatiotemporally heterogeneous processes in soft and disordered materials.

Acquisition to Reconstruction: 4D-STEM Tomography of Thick Biological Specimens

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Cryo-electron microscopy is the method of choice for biological imaging, but its applicability becomes increasingly limited for thick specimens because inelastic and multiple scattering compromise the projection approximation [1]. Four-dimensional scanning transmission electron microscopy (4D-STEM) combined with phase retrieval provides a promising route for tomography in this thickness regime. We collected 4D-STEM tilt series from specimens 200–700 nm thick, comparing ptychographic and tilt-corrected bright-field STEM (tcBF/parallax) reconstructions [2,3,4].

Several practical challenges arose during these reconstructions. Specimen tilt introduces a varying defocus across the field of view, which without dynamic defocusing during acquisition must be corrected computationally, either by choosing a single optimal defocus for parallax, or by varying the probe defocus as a function of scan position in the ptychographic forward model. Both approaches improve reconstruction quality but have limited effectiveness at high tilt angles, where hardware-level defocus correction becomes necessary. Additionally, multi-slice ptychography, despite its theoretical advantages [2], converged inconsistently at the single-digit e-/Å2 doses typical of cryo-tomography. Parallax proved more robust under these conditions and yielded tomograms from which preliminary sub-tomogram averaging shows encouraging results. We discuss strategies to address these challenges.

High Performance Computing and Artificial Intelligence Enabled Materials Characterization and Experimental Automation

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The capabilities provided by next generation light sources along with the development of new characterization techniques and detector advances are revolutionizing materials characterization (metrology) by providing the ability to perform scale-bridging, multi-modal materials characterization under in-situ and operando conditions. For example, providing the ability to image in 3D large fields of view (~mm3) at high resolution (<10 nm), while simultaneously acquiring information about structure, strain, elemental composition, oxidation state, photovoltaic response etc.

However, these novel capabilities dramatically increase the complexity and volume of data generated. Conventional data processing and analysis methods become infeasible in the face of such large and varied data streams. The use of AI/ML methods is becoming indispensable for real-time analysis, data abstraction and decision making at advanced, high-data rate instruments. I will describe how high-performance computing (HPC) along with AI on edge devices enables real-time data analysis and self-driving experiments, creating the next generation of AI-powered materials characterization tools.

As instrument and analysis workflows increase in complexity, large language models (LLM) have the potential to assist and enhance the productivity of scientists. I will describe early experiments with AI-powered scientific co-pilots that can provide assistance through every stage of an experiment; planning, execution, analysis and even instrument operation.

Exploring Neural Representations for 3D Phase Retrieval in Bragg CDI

Donghun Ryu[1], **David Simonne**[1], **Sayantan Mondal**[1], **Ericmoore Jossou**[1]
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Reconstructing three-dimensional crystal structures from intensity-only measurements remains a central challenge in coherent imaging, where missing phase information makes reconstruction highly ill-posed and sensitive to noise, initialization, and prior assumptions. These difficulties become especially pronounced in Bragg coherent diffraction imaging (BCDI) and related measurements involving complex phase variation, imperfect support estimates, and experimental aspects such as various noise sources and non-ideal illumination. In recent years, the powerful representation capabilities of neural networks have been exploited to improve the robustness of phase retrieval while preserving physical consistency.

In this work, we explore a neural framework that combines implicit priors with differentiable forward modeling to learn the underlying distribution of intensity measurements, enabling robust BCDI reconstruction without relying on accurate support constraints. By embedding measurement physics directly into the optimization process, our approach utilizes these continuous learned representations as an implicit regularizer. We will discuss diverse 3D phase retrieval results across various simulated sample geometries and phase complexities. We also compare our method against existing approaches, including classical iterative solvers, convolutional neural networks, and recent diffusion-based priors, including a comprehensive noise analysis. Beyond Bragg imaging, we expect our approach to have practical implications for other phase-sensitive microscopy modalities, where inverse reconstruction remains a major computational challenge.

Live ptychography reconstruction based on Holoscan platform toward autonomous feature detection and multimodal scans

Takenori Shimamura[1], *Zirui Gao, Ajith Pattammattel[1], Seher Karakuzu[1], Dmitri Gavrilov[1], Denis Leshchev[2], Yevgen Matviychuk[1], Garrett Bischof[1], Daniel Allan[1], Xiaojing Huang[1], Randy Smith[1], Adam Thompson[2], Stuart Wilkins[1], Yong Chu[1], Hanfei Yan[1]*
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Ptychography is a coherent diffractive imaging technique that quantitatively reconstructs the amplitude and phase information of samples using an iterative phase retrieval algorithm applied to multiple diffraction patterns. While this technique can achieve nanoscale resolution and high sensitivity, its measurement throughput is fundamentally limited by the acquisition speed of large volumes of diffraction data and the computational cost of the iterative reconstruction process. Live ptychography reconstruction can reduce the overhead associated with post-scan reconstruction by enabling simultaneous data acquisition and reconstruction [1], significantly expanding its application for in-situ and operando investigations. In addition, it facilitates rapid decision-making for subsequent high-resolution scans by instantly providing a reconstructed overview image of the sample [2].

To reduce scan downtime caused by iterative computation and manual decision-making, we are developing a live ptychography reconstruction pipeline [3] followed by automated feature detection at the Hard X-ray Nanoprobe beamline of the National Synchrotron Light Source II [4]. Live reconstruction is implemented using the NVIDIA Holoscan platform, which parallelizes modular tasks such as receiving diffraction-pattern streams from the detector, data preprocessing, and ptychographic reconstruction. Shortly after the detector starts acquiring images for the overview scan, the Holoscan-based application initiates the iterative ptychography reconstruction and continuously updates the results with the arrival of additional datasets. The live-reconstructed image is then processed by OpenCV-based feature detection algorithms to identify regions of interest for subsequent high-resolution zoom-in scans. These high-resolution scans are triggered according to their priority immediately after the overview scan.

Because this framework can be extended to other imaging techniques that require preprocessing, computational analysis, and visualization, we are also applying it to fluorescence detection combined with peak fitting and artificial-intelligence-based feature recognition. In this presentation, we will demonstrate the combined live-reconstruction implementation using battery particles and show results of crack, edge, and chemical-element-specific detection. This development will pave the way toward automated multimodal nanoscale imaging for operando setups.

Oral Presentation #34

Oral Presentation #35

Nano-Holotomography with Coded Apertures: From Simulation to Processing Large Experimental Data

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High-resolution phase-contrast 3D imaging via nano-holotomography conventionally requires tomographic data collected at multiple sample-to-detector distances. Beyond the fundamental limitation this imposes on temporal resolution, physically shifting the sample along the beam introduces algorithmic challenges in implementing accurate data scaling. To overcome this, we recently proposed a novel single-distance approach in which a coded aperture is synchronously shifted with sample rotation to introduce angle-dependent beam illumination across projections. The proposed approach was validated on simulated data, with results showing reconstruction quality matching the multi-distance approach while requiring only a single sample-to-detector distance and fewer total projections.
Although the potential of this approach was clearly demonstrated in our prior work, three limitations are addressed here. First, the probe function, coded aperture's transmittance function, aperture shifts, and shifts in object position were assumed to be known for simplicity. Second, the joint inverse problem was solved with the Alternating Direction Method of Multipliers (ADMM), which decomposes the objective into coupled subproblems that must each be solved at every iteration, incurring computational overhead and slow convergence. Third, validation was performed solely on synthetic data, leaving experimental validation of the approach untested. In this work, we address all three limitations as follows: (i) we lift the simplifying assumption by jointly recovering the probe, coded aperture transmittance, aperture shifts, and shifts in object position alongside the object's complex refractive index; (ii) we replace ADMM with a Conjugate Gradient (CG) method that exploits second-order curvature information via the bilinear Hessian framework recently developed by our group; and (iii) we demonstrate the proposed approach on experimental data acquired at beamline ID16A of the European Synchrotron Radiation Facility. Together, these advances establish the proposed method as a practically deployable and experimentally validated technique for dynamic, single-distance phase-contrast 3D nano-imaging.

Non-monotonic speckle contrast under micron-scale coherent illumination in wide-angle Bragg scattering

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Speckle contrast and size are key observables in coherent X-ray scattering experiments. While their dependence on experimental parameters is well understood in small-angle scattering and in under-sampled speckle regimes, their behavior in wide-angle geometries under tightly focused beams remains less explored.

We investigate speckle statistics at the specular Bragg peak of an exfoliated 1T-TaS2 flake as it is scanned through the focus of a coherent Gaussian X-ray beam at the EuXFEL MID beamline. The beam footprint depends on the distance between the sample and the optical focus. Crucially, the larger beams are not at the Gaussian focus of the focused X-ray spot. Across this focal series, the footprint is reduced from 30 μm to 0.5 μm. We observe a non-monotonic evolution of speckle contrast: it increases up to a 2.5 μm focal spot, then decreases at 0.5 μm. This reduction occurs even though the speckle size remains well oversampled relative to the detector pixel size. Simultaneously, the speckle shape becomes anisotropic due to the projection of the beam footprint in Bragg geometry.

The evolution of speckle size and contrast is quantified using speckle autocorrelation and speckle visibility analysis. To interpret the observations, we perform forward modeling of the scattered wavefront using experimentally constrained parameters including domain morphology and the number of scattering features within the illuminated volume. The projected beam footprint on the sample becomes compressed or stretched along the scattering plane depending on the incident and exit angles, producing anisotropic speckles and modifying the number of contributing scatterers.

These results reveal an overlooked mechanism governing speckle contrast in the oversampled speckle regime and highlight the role of focused beam size and scatterer statistics in wide-angle XPCS experiments. Our findings provide guidance for optimizing speckle contrast in experiments using micron-scale focused coherent X-rays at modern synchrotron and free-electron laser facilities.

Progress and Current Status of Diamond Lenses for X-Ray Focusing

Sergey Antipov[1]
[1]PALM Scientific

Diamond lenses are becoming increasingly important for modern x-ray optics because diamond offers a unique combination of high thermal conductivity, low thermal expansion, excellent radiation hardness, and exceptional suitability for high-power x-ray focusing. These properties make diamond especially well suited to the demands of synchrotrons and free-electron lasers, where optical elements must maintain stability and performance under intense heat loads. Today, hundreds of diamond lenses manufactured by PALM Scientific are deployed at synchrotron facilities around the world, demonstrating both the maturity of the technology and its growing adoption.

This presentation will review the current status of diamond lens technology, with emphasis on practical manufacturing capability and application readiness. We will summarize the lens geometries that are currently achievable, including the dimensional and form accuracy that can be obtained in production. We will also discuss which geometries are polishable and which are limited by material, access, or other fabrication constraints. Particular attention will be given to the tradeoffs between optical design freedom, manufacturability, and achievable surface quality.

In addition, we will present current packaging approaches for both individual diamond lenses and compound refractive lens (CRL) assemblies. These options are important for alignment, robustness, handling, and integration into beamline systems. By reviewing geometry, accuracy, "polishability", and packaging together, this talk provides an updated picture of the current state of diamond lens technology and the pathways for further improvement and broader deployment.

Precision Laser Machining for Applications at Light Sources

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Laser microfabrication enables geometries, features, and surface finishes that are difficult or impossible to achieve with conventional machining, creating new opportunities for scientific instrumentation and high-pressure research. This poster will review applications of precision laser machining for the scientific community, with examples drawn from work performed by PALM Scientific, a company founded to provide custom laser microfabrication services for researchers.

A primary focus will be on diamond anvil cell components. Examples will include diamond anvil perforation for reducing x-ray absorption, as well as polishing methods that preserve the optical quality needed for ruby fluorescence pressure measurements. The presentation will also discuss diamond anvil culet shaping, including designs intended to reduce sample slippage during dynamic compression and geometries that improve gasket placement and sample control. These cases illustrate how laser processing can directly improve experimental performance, alignment, and measurement reliability.

Additional applications to be reviewed include fabrication of diamond x-ray lenses, glassy carbon refractive lenses, tungsten masks for x-ray, laser, and electron-beam systems, custom-machined fluorescence screens, and diamond membranes. Together, these examples demonstrate the flexibility of laser microfabrication as a tool for producing specialized components for demanding scientific experiments. The goal of this presentation is to show how close collaboration between researchers and a precision laser machining vendor can accelerate development of custom solutions for advanced scientific applications.

Atomic (34-ID-F): New Home of Bragg Coherent X-ray Diffraction Imaging

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Taking advantage of the high coherence and brightness of the third-generation synchrotron source, 34-ID-C of the Advanced Photon Source (APS) provided detailed local structural information at nanoscale and its evolution of crystalline materials in 3D. The usage of modest X-ray optics with relatively long working distance enabled in-situ/operando experiments employing Bragg coherent X-ray diffraction imaging (BCDI) to address scientific questions on various materials.

The high coherent flux from the upgraded APS (APS-U) will enable a revolution in BCDI. The new Atomic (34-ID-F) beamline at Sector 34, a feature beamline of the APS-U, will take full advantage from the APS upgrade. One anticipates that 3D imaging at the Atomic beamline approaches ultimate spatial resolution in some experimental cases and achieves much higher temporal resolution than what was available at the APS in others. In this presentation, I will discuss the future of BCDI as well as the development at the Atomic beamline of the APS-U.

From SPring-8 to Global Deployment: System-Level Adaptation of the CITIUS Detector for Coherent X-ray Beamlines

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Advances in coherent X-ray sources require detector technologies that combine high dynamic range, fast readout, and fine pixel pitch. The CITIUS detector system, developed at RIKEN and deployed at SPring-8, has demonstrated strong performance in coherent diffraction imaging, ptychography, and time-resolved experiments. Its integrating-type pixel architecture provides precise charge collection, low cross-talk, and robust operation across broad photon energy and flux ranges, enabling accurate measurement of weak interference features alongside intense primary beams.

Building on these successful results at SPring-8, kai scientific Ltd. is leading efforts to deploy the CITIUS detector technology to other synchrotron and free-electron laser facilities worldwide while maintaining its demonstrated performance and improving reliability. Deployment at facilities other than SPring-8 requires system-level adaptation to diverse beamline environments.

CITIUS's standard frame rate of 17.4 kframes/s makes individual frame triggering impractical, as it would introduce inter-frame latency. To address this constraint, the detector operates at the "train" level, where each train contains a predefined number of native frames, typically 5000 frames per train. Train triggers, typically generated within the system, initiate frame sequences with deterministic timing and high temporal precision. This acquisition concept enables stable operation at high repetition rates.

A further consideration is data bandwidth. CITIUS generates 1.7 PB/day of data even for the minimum 280 kpixel system. To facilitate data handling, the system is equipped with Edge servers incorporating FPGA-based Data Framing Boards, which perform real-time calibration, frame accumulation, and structured data reduction prior to storage. This hardware-accelerated processing significantly mitigates data throughput while preserving the high dynamic range and temporal fidelity required for coherent X-ray measurements.

This contribution will describe the CITIUS detector system architecture, its adaptation for deployment beyond SPring-8, and recent implementation examples demonstrating suitability under diverse beamline conditions. Scalability options, including in-vacuum configurations and larger camera head variants, will also be discussed in the context of future global deployment.

AEON: Large-Area Timepix4 Detector by X-Spectrum

Svenja Hovelmann, **Alexander Ignatenko**, *Jorn Lange, Dara Marin, Julian Schmehr, Sergei Smoljanin, Jonas Warias*

The demand for high-resolution, time-resolved detection in synchrotron and XFEL experiments motivates the development of advanced, large-area detector systems. AEON, developed by X-Spectrum, is a scalable detector platform based on the Timepix4 ASIC, designed to combine the fine spatial resolution of 55 µm pixels with precise timing in a large-area format, while supporting higher frame rates than its predecessors.

AEON can operate in an event-driven readout mode, enabling simultaneous measurement of time-of-arrival (ToA) and time-over-threshold (ToT), providing per-photon timing and energy information. A frame-based acquisition mode is under development to further expand operational flexibility. The frame rates will reach up to 40 kHz at 8-bit and up to 20 kHz at 16-bit resolution. The modular detector architecture allows tiling of multiple Timepix4 chips to achieve large sensitive areas with minimal dead space.

X-ray Photon Correlation Spectroscopy (XPCS) experiments were carried out at the P10 beamline of PETRA III, ID10 at ESRF, and APS. Each beamline presented different synchrotron bunch structures, and all of them were clearly resolved with the detector. The setup enabled the measurement of sample dynamics down to sub-µs timescales. For 9.6 keV photons, a time resolution of 8.3 ns was achieved, currently limited by the silicon sensor response.

The advantages of employing event-based detection for time-resolved synchrotron experiments are highlighted by laser pump - X-ray probe diffraction experiments at XPP@KMC-3 BESSY II. The detector has demonstrated the capability to resolve the complex bunch filling patterns employed by BESSY II. The high time resolution allows for efficient data collection even with tightly spaced bunch structures. The detector allows for the analysis of both short- and long-timescale excitation and relaxation processes within a single measurement, exhibiting a favorable signal-to-noise performance.

Development and Current Status of CITIUS Detectors for X-ray Coherent Applications

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Coherent X-ray experiments generally require detectors capable of achieving high frame rates, low noise, and the ability to sustain high photon flux in order to accurately record speckle patterns over time. To address these requirements, we have developed the CITIUS detector family, an integrating-type pixel detector optimized for high-flux coherent X-ray measurements.

The detectors are based on a novel pixel structure that enables low leakage current and low-noise operation, coupled with high-speed parallel readout electronics and FPGA-based real-time data processing. In this contribution, we present the novel pixel design and discuss how radiation hardness, gain stability against radiation exposure, and low leakage current are achieved through the sensor architecture.

The CMOS sensor integrates 36,864 on-chip ADCs, with one ADC serving eight pixels, enabling massively parallel signal digitization. A gain selection scheme is adopted to avoid the instantaneous global cross talk typically associated with gain switching. In this architecture, both the high-gain and medium-gain signals are digitized by the on-chip ADCs, and the appropriate gain value is selected at the chip periphery in the digital domain before transmission off-chip. While this approach suppresses cross talk at the architectural level, it is not advantageous in terms of frame rate because multiple gain channels must be digitized. The required high frame-rate operation is nevertheless achieved by implementing a large number of ADCs on the chip, enabling highly parallel readout.

We also present detector performance demonstrated in recent ptychography experiments and in deployments for X-ray photon correlation spectroscopy (XPCS). In addition, the development status of a 5.04-Mpixel CITIUS detector, planned for deployment in September 2026, will be introduced.

Poster Presentation #43

The Sector for Coherent High Energy X-ray studies (CHEX) at the Upgraded Advanced Photon Source

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The Advanced Photon Source (APS) at Argonne National Laboratory has recently completed an upgrade, resulting in an approximately 100-fold increase in the coherent flux of the X-ray beam. This significant enhancement presents new opportunities to utilize coherent scattering techniques such as X-ray Photon Correlation Spectroscopy (XPCS) and Coherent Diffraction Imaging (CDI) at high X-ray energies, which can penetrate complex sample environments. This advancement will enable a new class of in-situ studies across a wide range of disciplines. As part of the APS upgrade, nine feature beamlines are being built with unique capabilities designed to take advantage of the upgraded X-ray source. I will describe the new feature beamline at Sector 28 for Coherent High Energy X-ray Studies (CHEX), designed with an emphasis on in-situ and in-operando studies. This description will include details on CHEX's multiplexed design, which, when fully operational, will allow for four experiments to be performed simultaneously, as well as its infrastructure for accommodating large and complex sample environments.

High-Energy Coherent X-ray Approaches for In Situ and Operando Studies of Energy Materials at the CHEX Beamline

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The Advanced Photon Source Upgrade (APS-U) includes several featured beamlines designed to exploit the high coherent flux available from the upgraded storage ring. One of these is the Coherent High-Energy X-ray (CHEX) beamline, which focuses on coherent scattering experiments at high photon energies (typically ~10–75 keV). These energies enable measurements in in situ and operando environments, as the increased penetration of high-energy X-rays allows experiments through realistic sample environments, reaction cells, and windows.

Building on these capabilities, we discuss opportunities enabled by the CHEX beamline for coherent X-ray studies of energy materials, particularly electrochemical systems and heterogeneous catalysis. One major application area is the operando investigation of battery materials, where the high-energy beam enables coherent X-ray measurements of active materials embedded within complex cell architectures. Techniques such as Bragg coherent diffraction imaging (BCDI) and X-ray photon correlation spectroscopy (XPCS) provide access to strain evolution, structural heterogeneity, and dynamic processes during electrochemical reactions. Heterogeneous catalysis represents another important application area, where coherent scattering methods can be used to investigate structural evolution and nanoscale dynamics of catalyst particles under reaction conditions.

Electrode surfaces in electrochemical systems and catalytic interfaces represent another important target for the CHEX beamline. In addition to established surface-sensitive methods such as X-ray reflectivity (XRR) and crystal truncation rod (CTR) scattering, coherent surface scattering approaches will be developed to enable measurements such as single-shot ptychographic imaging and time-resolved studies of interfacial fluctuations and reaction dynamics using XPCS. Ultimately, these approaches aim to visualize chemical and electrochemical reactions occurring at surfaces, together with the associated surface reconstructions, with nanometer-scale spatial resolution and time-resolved evolution approaching nanoscale "movies" of interfacial processes.

By combining high-energy coherent X-rays with in situ and operando environments, the beamline aims to enable new experimental approaches for studying energy materials across multiple length and time scales.

Poster Presentation #45

The In-Situ Nanoprobe Beamline at the Upgraded Advanced Photon Source

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The In-Situ Nanoprobe (ISN) is a feature beamline of the recently upgraded Advanced Photon Source, designed to deliver a fully coherent, sub-50 nm x-ray beam with a large working distance. This combination enables flexible integration of diverse sample environments and detection modalities, supporting a broad range of in situ and operando experiments. We present an overview of the beamline design and performance, highlight key capabilities and experimental opportunities for users, and share preliminary scientific results demonstrating the potential of ISN.

Poster Presentation #46

Bragg Coherent Diffraction Capability at the Advanced Photon Source High-Energy X-Ray Beamline HEXM

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The recent Advanced Photon Source (APS) upgrade offers significantly improved coherence properties at higher x-ray energies (> 40 keV), enabling Bragg coherent diffraction imaging (BCDI) of individual grains in materials as an additional investigative zoom-in technique to an existing set of high-energy x-ray diffraction microscopies on polycrystalline systems. The long beamline HEXM (High-Energy X-Ray Microscope) was built as a featured part of the APS-upgrade to exploit the enhancement of these applications. The BCDI implementation scheme at HEXM will be presented, including the optical layout [1] for longitudinally and transversely coherent beams for large grains of interest, the sample manipulation system, and the distant detectors to record finely-spaced diffraction fringes. Some first measurements will be shown, along with exploratory development done earlier at the high-energy beamline 1-ID.

Poster Presentation #47

Study on precise alignment of sub-10 nm X-ray nanofocusing mirror system

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The upgrade of the SPring-8 storage ring to the diffraction-limited source SPring-8 II will significantly increase the brightness and transverse coherence of hard X-ray beams while reducing the effective source size (Tanaka et al., 2024). These improvements make sub-10 nm X-ray nanofocusing with high photon flux feasible. Among various focusing optics, Advanced Kirkpatrick-Baez (AKB) mirrors based on the Wolter III geometry are promising because they enable a large demagnification required for nanofocusing while maintaining high reflectivity through total reflection, and near diffraction-limited focusing has been demonstrated (Yamada et al., 2019).

However, achieving sub-10 nm focusing in practice remains challenging, as it requires extremely precise mirror alignment, a high-precision mirror manipulator, and excellent mirror figure accuracy.

In this work, we develop a sub-10 nm X-ray focusing optical system based on Wolter III AKB mirrors. The optical design parameters were optimized to provide a large demagnification factor on the order of 10^4, targeting ~7 nm high-flux focusing of a 21 keV X-ray beam with an expected photon flux of up to 10^{13} photons/s for the upcoming SPring-8 II upgrade.

To realize the designed optical performance, wave-optical calculations were first performed to evaluate the mirror alignment tolerances of the optical system. Alignment experiments were carried out at BL29XUL of SPring-8 using the high-precision mirror manipulator developed in this work. The mirrors were initially coarsely aligned to the designed geometry and further optimized using wavefront measurements with a grating interferometer (Yamada et al., 2020) to quantitatively evaluate and correct alignment errors, resulting in improved focusing performance.

The results demonstrate that the alignment strategy provides an effective approach for optimizing sub-10 nm X-ray focusing optics, enabling quantitative analysis of wavefront aberrations and mirror figure errors for further refinement of the optical system.

Revealing mechanisms of processing defect mitigation in laser powder bed fusion via shaped beams using high-speed X-ray imaging

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The laser powder bed fusion (LPBF) process utilizing a focused Gaussian-shaped beam faces challenges, including pore formation, melt pool fluctuation and liquid spattering. While beam shaping technology has been explored as a potential approach for defect mitigation, the beam-matter interaction dynamics during melting with shaped beams remains unclear. Here, we report the direct observation of ring-shaped beam-matter interaction dynamics, including pore formation, melt pool fluctuation and liquid spattering, and unveil defect mitigation mechanisms in ring-shaped beam laser powder bed fusion process. We find that, by spatially manipulating incident laser rays, the ring-shaped beam controls keyhole morphology, thereby managing the redistribution of the reflected rays. This manipulation can effectively eliminate the formation of an unstable cavity at the keyhole tip, stabilizing the keyhole and mitigating keyhole pores. This enhanced keyhole stability effectively reduces the melt pool fluctuation, the formation of liquid breakup induced spatters and liquid droplet colliding induced large spatters in the laser powder bed fusion process. Additionally, the high-energy forefront of the ring-shaped beam effectively melts the powder bed, reducing agglomeration liquid spatter in the laser powder bed fusion process. The discovered defect mitigation mechanisms may guide the design of beam shaping strategies for simultaneously increasing the quality and productivity of metal additive manufacturing.

Coherent O-K-Edge Imaging of Tantalum Films Relevant to Millisecond-Lifetime Qubits

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In the last four years, the qubit lifetimes of 2D transmon superconducting qubits have improved nearly 30 fold, reaching T1 values approaching 2 ms [1,2] and opening the door to practical quantum applications. These gains are largely attributed to improvements in metal selection for resonator pads, control of the air–metal–oxide–metal interface, and careful preparation of the substrate surface prior to metal deposition.

A recent in depth study of a series of tantalum films deposited on sapphire revealed two distinct performance classes, despite all films exhibiting high internal quality factors (Qint ~1×10^6 to >1×10^7). To investigate the material origins of this performance split, we used coherent soft REXS at the CSX beamline to perform real space spectral imaging across the O K edge on patterned Ta films. These measurements leveraged a new low noise, large area detector [5] that offers substantially improved spatial resolution compared with the previously used FastCCD; for comparison, we will also present down sampled data to illustrate this improvement.

Between the two Ta film classes, we observed surfaces structures comparable to atomic force microscopy (AFM) results, but with the added advantage of oxygen sensitivity. Full field, real space spectral imaging—with zoom and position control—may offer a superior and faster method for evaluating surface oxidation and associated morphologies than the combined results from AFM and surface averaged X ray photoelectron spectroscopy [1,3,6]. Such spatially and chemically specific insight is essential for advancing the fabrication of world leading qubits.

Present and Near-Future Coherent Imaging Capabilities at National Synchrotron Light Source II

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[1]National Synchrotron Light Source II

National Synchrotron Light Source II (NSLS-II) has significant coherent imaging capabilities with a broad range of scientific applications. High-speed ptychographic imaging is a part of the multimodal imaging pipeline of the Hard X-ray Nanoprobe (HXN) beamline, which includes fluorescence, diffraction, and spectroscopic (XANES) imaging modalities using a sub-15 nm x-ray beam. Coherent Diffractive Imaging (CDI) beamline, optimized for Bragg CDI, is presently under commissioning. Soft X-ray Nanoprobe (SXN) beamline, operating over 0.25-2.5 keV, will offer the conventional scanning transmission x-ray microscopy capability with sub-20 nm resolution, along with ptychographic imaging capability aiming at a spatial resolution down to 2 nm. SXN is expected to begin commissioning in Spring, 2027. Advanced Nanoscale Imaging (ANI) beamline (operating over 6-25 keV) and Tender X-ray Nanoprobe (TXN) beamline (operating over 1-14 keV), to be completed in 2032, will offer optimized for ptychography imaging with a long working distance, while still offering multimodal imaging capabilities with fast switching between scanning and full-field imaging modes. ANI and TXN will have an automatic sample exchanger for loading multiple samples into their endstation vacuum chamber and a significant sample- to-detector distance up to 10 m. ANI will provide 3D imaging under the laminography geometry, offering efficient 3D imaging for samples with planar interfaces such as microelectronics devices on Si wafers. The presentation will give technical details on these advanced beamlines, making connections to their scientific applications.

Dichroic Coherent Diffraction at the POLAR Beamline

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[1]APS/ANL

The recent completion of the upgrade has opened outstanding opportunities for the user community at the Advanced Photon Source at Argonne National Laboratory. The new low emittance x-ray source is now providing brilliant and highly coherent beams, allowing for exciting experimental possibilities in scattering and spectroscopy in the hard x-ray range. POLAR, the beamline for polarization modulation spectroscopy at sector 4 of the APS [1], is utilizing intense focused beams with a high degree of coherence and tunable polarization. Researchers have access to a variety of sample environments, such as for variable temperature, high magnetic fields, extreme pressures, and uniaxial strain, to combine with the beamline's advanced focusing capabilities and energy tunability.

The flexible imaging and scattering setup features KB focusing optics, a nanopositioning stage, and an Eiger X 1M pixel array detector, together with phase-retarder optics for variable incident polarization, enabling dichroic coherent diffraction experiments. Interferometers are used to monitor the sample position. Thus, the new beamline supports experiments based on dichroic ptychography, 3D dichroic tomography [2], and Bragg coherent diffraction, allowing studies of magnetic or electrically polarized textures within the bulk of materials.

We will present initial results on dichroic imaging and discuss future opportunities and planned upgrades to incorporate low-temperature and magnetic-field capabilities into the imaging setup.

An Efficient Wave-Optics Framework for Partially Coherent Pink X-ray Beam Simulation and Analysis

Ming Li, **Shuo Wang**, *Han Xu, Liang Zhou*

Fourth-generation Synchrotron Radiation Sources provide highly coherent X-ray beams for coherent diffraction imaging, ptychography, and X-ray photon correlation spectroscopy, but many experiments remain photon limited. Pink-beam operation can substantially increase flux by accepting a finite bandwidth; however, quantitative prediction of partial coherence, chromatic aberration, and broadband wave-optics propagation remains computationally challenging. Here we present an efficient wave-optics framework for simulating and analyzing partially coherent pink X-ray beams. The framework combines Monte-Carlo Brightness Convolution for efficient wavefront-matrix construction, Hierarchical Incremental Singular Value Decomposition for memory-efficient coherent-mode decomposition, and spectral-spatial decomposition for rapid propagation of broadband coherent modes.

The method is benchmarked using simulations and measurements from the HEPS Hard X-ray Coherent Scattering beamline. For a single-energy 12.4 keV source, the proposed approach reproduces SRW-calculated intensity distributions, coherent modes, and spectral degree of coherence while completing coherent-mode analysis in about 14 minutes with 5.09 GB peak memory on a personal computer. Broadband simulations over 50 photon-energy points were completed in about 71 minutes on 50 CPU cores. The propagated wavefronts were further validated against fluorescence-screen measurements at HEPS HXCS at 12.40 and 12.20 keV. We then applied the framework to compound refractive lens focusing under pink-beam operation. Compared with the quasi-monochromatic central cone, the pink beam broadened the simulated focus from 15.6 um x 9.0 um to 19.8 um x 11.2 um and reduced the coherent fraction from 50.84% to 44.83%. This scalable framework provides a practical tool for designing and interpreting high-flux coherent X-ray experiments using partially coherent pink beams.

Joint Holotomography Solver for Large-Scale Experimental Data Processing

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Multi-distance holotomography is a full-field phase-contrast X-ray imaging technique that combines phase retrieval with tomographic acquisition to reconstruct three-dimensional distributions of the complex refractive index. Using highly coherent hard X-ray beams from modern synchrotron sources, the method enables non-destructive nanoscale imaging of weakly absorbing specimens such as biological tissues and functional materials, with spatial resolutions routinely reaching the sub-100 nm range. As fourth-generation synchrotron sources further increase brightness and coherence, holotomography is being pushed toward even finer length scales. However, these improvements also increase sensitivity to experimental non-idealities, including structured illumination, positioning errors and sample instability. As a result, conventional reconstruction pipelines—typically composed of separate alignment, phase retrieval, and tomographic inversion steps—may introduce artifacts or reduce quantitative accuracy when underlying modeling assumptions are violated.

In this work, we present a practical joint reconstruction framework for large-scale multi-distance holotomography. Rather than solving individual subproblems sequentially, the proposed approach formulates holotomography as a single inverse problem in which the three-dimensional object, the illumination probe, and the scan-position errors are estimated simultaneously from the measured intensity data.

To make this approach computationally feasible for realistic synchrotron datasets, we introduce an efficient second-order optimization strategy based on the bilinear Hessian, which incorporates curvature information at a computational cost comparable to gradient-based methods. The algorithm is implemented in a scalable architecture combining chunked data processing, multi-GPU execution, and distributed-memory parallelism, enabling joint reconstruction of volumetric datasets exceeding thousands of voxels per dimension.

We validate the framework on experimental datasets acquired at ESRF beamline ID16A, including a three-dimensional resolution phantom and a mouse brain sample. The proposed method reduces probe- and alignment-related artifacts and yields improved reconstruction quality compared with conventional sequential beamline workflows, demonstrating the feasibility of joint reconstruction for routine high-resolution holotomography experiments.

A computational study for ultrafast x-ray photon correlation spectroscopy

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Ultrafast X-ray photon correlation spectroscopy (XPCS) has emerged as a unique capability enabled by X-ray free-electron lasers (XFELs). By measuring time-resolved coherent diffraction patterns, or speckle patterns, XPCS provides direct access to structural dynamics over a wide range of length and time scales, from atomic motion to nano- and micro-scale structural evolution. This capability makes XPCS a powerful tool for investigating diverse phenomena in materials science, including crystal growth dynamics, defect dynamics, and disorder-order phase transitions.

A particularly compelling application is the study of the glass transition and the dynamics of supercooled liquids. Despite significant progress in atomistic simulations over the past two decades, a fundamental gap remains between simulated quantities and experimentally accessible XPCS observables, limiting direct comparison.

Here, we propose a machine-learning framework for analyzing atomistic simulation data that bridges this gap by learning dynamical representations of liquid and glassy systems and predicting the corresponding temporal correlation functions measured in XPCS. This approach establishes a unified pathway for interpreting XPCS data, enabling quantitative comparison between simulation and experiment, and has the potential to provide new insights into the microscopic mechanisms underlying the glass transition.

Methodological Developments at the CDI Beamline of NSLS-II

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The Coherent Diffractive Imaging (CDI) beamline at 9-ID of the National Synchrotron Light Source II is currently under commissioning. The beamline is designed to provide novel controlled X-ray illumination, advanced sample environments, and flexible experimental geometries. While this state-of-the-art design enables unprecedented capabilities and flexibility for coherent diffractive imaging experiments, new methodologies are required to achieve accurate and efficient measurements that fully leverage these capabilities.

Here we present recent methodological developments at the CDI beamline, including a wave-propagation-based phase-retrieval workflow for Bragg coherent diffractive imaging and a machine-learning-based grain mapping method. The former builds on our recent work incorporating dynamical diffraction effects and non-trivial incident beam profiles into the forward simulation, enabling a backward-propagation reconstruction workflow. The latter provides an efficient approach to mapping grain sizes and orientations in three-dimensional polycrystalline samples by leveraging modern machine learning techniques.

Multi-beam STXM with a diffractive OSA

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We present results from proof-of-principle experiments which demonstrate multi-beam scanning transmission X-ray microscopy (STXM). Instead of creating multiple beams with lenses or zoneplates, we incorporate a grating into the the order sorting aperture (OSA). This grating-OSA performed two duties. Firstly, it acts as a conventional OSA by selecting a single order of the zoneplate. Secondly, the grating splits the zoneplate focus into several focii. STXM scans are performed in parallel allowing the beamline's photon flux to be utilized more fully. Each focii can have different properties depending on the structure of the grating. In these experiments, focii with different orbital angular momentum were produced using a forked grating. There is potential to use this method to extract additional sample information, such as helical dichroism. Comparisons between experimental measurements and simulations will be presented which show good agreement and support our understanding of the method.

Multiscale Mapping of Precipitate–Matrix Interactions in a Bulk Polycrystalline Material under In-Situ Tensile Loading via High-Energy Bragg Coherent Diffraction Imaging

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Deformation behavior in polycrystalline materials arises from complex hierarchical structure and interactions across multiple length scales. Accordingly, a range of X ray methods—spanning wide angle X ray scattering, high energy X ray diffraction microscopy (HEDM), and Bragg coherent diffraction imaging (BCDI)—have been developed to probe deformation across length scales. A central objective is to establish quantitative links through these multi-scale measurements to elucidate the fundamental mechanisms governing mechanical interactions in polycrystals.

Here, we investigate precipitate–matrix interactions and the resulting intragranular lattice distortion within individual precipitate grains using a multiscale, in situ X ray diffraction imaging approach at Advanced Photon Source (APS), Argonne National Laboratory. Specifically, we employ HEDM and Bragg coherent diffraction imaging (BCDI) in a unified instrument to connect grain scale mechanics to nanoscale strain and displacement fields in deeply embedded σ phase precipitates within the austenitic γ matrix of polycrystalline 316 stainless steel (SS316). In SS316, the σ phase is brittle and poorly coherent with the γ matrix, thereby degrading strength and life by acting as a crack initiation site.

The high coherence and brightness of the APS Upgrade source enable high resolution BCDI measurements in bulk polycrystalline specimens. HEDM is first used to map grain orientations and diffraction reflections to identify and select suitable precipitate targets for subsequent BCDI measurements. BCDI then reconstructs the three dimensional morphology along with displacement of individual σ precipitates from multiple Bragg reflections with high sensitivity. During in situ mechanical loading, evolution in the positions and shapes of the BCDI diffraction patterns is tracked to quantify the evolving mechanical response of the corresponding precipitate grains. In parallel, we characterize the grain resolved response of the surrounding γ matrix to determine how stress concentrates around σ precipitates, how cracks nucleate and initiate growth within σ, and how damage transfers into the matrix.

Robust Algorithms for the Next Generation of Bragg Coherent Diffraction Imaging

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In just the past few decades, the technique known as Bragg coherent diffraction imaging (BCDI) has grown from an interesting thought experiment into a promising new form of structural microscopy. Unfortunately, this progress is increasingly challenged by practical constraints. For example, improvements to synchrotrons around the world allow scientists to measure larger regions of reciprocal space, where signal would previously have been too faint. Such measurements should produce images with unprecedented resolution. However, increasing the detection volume also increases the chance that any other grain caught in the beam will cast its own Bragg reflection onto the detector, corrupting the intended measurement. As a result, the best BCDI-produced images often depict isolated nanocrystals which do not necessarily represent the properties of bulk materials. The next generation of BCDI will require more robust reconstruction algorithms to handle these and other practical challenges. In this poster, we present such an algorithm, which leverages the redundancy of multiple Bragg peaks from a single source to detect and remove the influence of spurious measurements over the course of a reconstruction. We show that, compared to manual removal of these artifacts, this algorithm produces more accurate images and removes the need for time-consuming, expert-dependent intervention before reconstruction.

Live Reconstruction for Bragg Coherent Diffraction Imaging During Data Acquisition

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Bragg coherent diffraction imaging (BCDI) is a powerful technique for reconstructing three-dimensional crystal morphology and lattice displacement fields from coherent x-ray diffraction measurements. The technique has enabled operando studies of nanoscale structural evolution in crystalline materials, including crystal growth and dissolution, electrochemical cycling in battery materials, catalytic reactions, and thermally driven phase transformations, where lattice strain and defect dynamics evolve under working conditions.

However, conventional BCDI image reconstruction is performed after the full reciprocal space dataset has been acquired, limiting live feedback during experiments and often leading to inefficient scan strategies and unnecessary radiation exposure, particularly at high-brilliance synchrotron sources.

In this work, we present a live reconstruction framework for Bragg coherent diffraction imaging in which three-dimensional reconstructions of crystal support, morphology, and displacement field are computed concurrently with data acquisition. The method reconstructs the image by sequentially incorporating diffraction slices as they are measured, enabling continuous updates to the reconstructed image throughout the duration of the measurement.

Real-time image reconstruction enables new measurement strategies, including immediate assessment of reconstruction quality, early termination of scans once sufficient image fidelity is achieved, and dynamic adjustment of scan parameters during the experiment, particularly for measurements that are sensitive to radiation dose or require rapid time resolution. More broadly, this framework transforms BCDI from a post-processing technique into an interactive imaging method, where experimental parameters such as applied load, temperature, electrochemical potential, or liquid and gas environments can be modified in response to the evolving reconstructed image during the experiment.

Correlating the strain distribution and plasticity in a layered chiral magnet using symbolic regression

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Quasi-two-dimensional (quasi-2D) materials host mechanical, electrical, and magnetic properties useful for novel microelectronic devices. Of particular interest are quasi-2D chiral magnets which are a much-desired platform for new topological spin structures and related transport phenomena. Therefore, mapping and understanding the mechanical strain inherent or induced in quasi-2D materials accurately is critical to enhancing their functionality in devices.

We focus on the distribution of strain and sheer in an intercalated transition metal dichalcogenide (TMD) Cr1/3TaS2. Recent work on Cr1/3TaS2 demonstrated emergent spiral magnetic superstructures that can be directly affected by both the shear strain and the application of an external field as low as 100 Oe. Despite these observations, the connection between the magnetic spin and the lattice is yet to be experimentally explored.

We performed scanning x-ray nanodiffraction measurements of exfoliated Cr1/3TaS2 flakes. We collected five-dimensional dataset that was transformed into the intensity distribution in reciprocal space around the lattice vector at each probed location and used it to spatially resolve the distribution of εyz and εxz as the leading terms of the strain tensor. We then employed a symbolic regression methodology to select the outliers in terms of strain magnitude. Using a model trained on similar data, the model is used to quantify the plasticity of strain in the Cr1/3TaS2.

Towards reduced dose Hard X-ray imaging with correlated photons

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Despite wide-applicability and high potential resolution, Hard X-ray imaging on biological systems faces a severe shortcoming due to damage caused by ionizing radiation on the sample during exposure. Due to the ability to exploit correlations between imaging photons from the source, microscopies based on correlated or entangled Hard X-rays photons are promising avenues for reduced dose imaging. Here we present first steps towards the development of a quantum microscope through the investigation of spontaneous parametric down-converted (SPDC) photons in diamond single crystals at the Coherent Hard Scattering X-ray beamline (CHX) at NSLS-II.

Building on previous work where we have demonstrated ghost imaging using SPDC photons, we explore several geometries of SPDC photon generation in Bragg geometry using (111), (333), and (400) reflections at 15 keV, 12.77 keV, and 9.83 keV, and demonstrate the relative suppresion of elastic thomson scattering by the pump photons results in a higher SPDC signal to background ratio. These results aid the development of next generation hard x-ray microscopy for radiation sensitive samples by enabling careful choice of source parameters to minimize non-correlated photon radiation on the sample, and will assist in future Hard x-ray imaging with reduced radiative dose.

Poster Presentation #62

Bubble explosion induced melt pool instabilities in electron beam melting of aluminum alloy

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Electron beam melting (EBM) is an additive manufacturing technology that can process materials and manufacture components otherwise impossible or uneconomical. However, defects, including porosity and surface irregularities, are widely reported in EBM-built components, and their formation mechanisms are not fully understood. Here, using in-situ high-speed synchrotron X-ray imaging, we reveal that bubble explosions in Al6061 during EBM induce melt pool instabilities contributing to defect formation. The melt pool and keyhole evolve through three stages: (1) initial formation of a melt pool, (2) subsurface bubble formation and explosion, and (3) periodic keyhole oscillation. During scanning, periodic bubble explosions can eject molten liquid as spatters and disturb the vapor depression and melt pool, contributing to surface humping, that may trigger lack-of-fusion defects in subsequent layers. The physical insights we report could provide guidance for EBM machine development, process innovation, alloy design and model development.

X-FAST: XUV Femtosecond Absorption Spectroscopy Tabletop Facility at UW-Madison

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Transient absorption spectroscopy combined with an extreme ultraviolet (XUV) probe and a visible or infrared pump has emerged as a powerful approach for investigating ultrafast electronic dynamics in materials. By probing core-level transitions, XUV spectroscopy provides element-specific sensitivity, enabling direct observation of charge transfer, oxidation-state changes, and electronic structure evolution on femtosecond timescales. This capability is particularly valuable for complex materials composed of multiple elements, where disentangling site-specific dynamics is essential for understanding their functional properties.

Recent advances in tabletop high harmonic generation (HHG) have enabled the production of broadband XUV radiation in laboratory environments, making core-level transient absorption spectroscopy accessible beyond large-scale facilities. Using this approach, we commissioned the X-FAST (XUV Femtosecond Absorption Spectroscopy Tabletop) facility at the University of Wisconsin–Madison. This system combines a femtosecond optical pump with an HHG-generated XUV probe spanning approximately 40–70 eV, enabling element-resolved measurements of ultrafast processes in thin films and functional materials.

Initial experiments with the X-FAST setup have focused on transition-metal-based materials where coupled electronic, structural, and magnetic degrees of freedom play a critical role. In particular, studies on the Heusler alloy Ni_2MnGa have explored ultrafast dynamics near the Mn and Ni ($M_{2,3}$) absorption edges, providing insight into femtosecond electronic responses associated with structural distortions and phase transitions. Complementary investigations on MnPtGa further demonstrate the capability of XUV transient absorption to probe element-specific charge transfer and electronic redistribution in complex magnetic materials.

Together, these studies highlight the versatility of the X-FAST instrument for probing ultrafast processes in magnetic alloys and multifunctional materials with high temporal and element specificity.

X-Ray Phase-Contrast Imaging Time Evolution of Shock-Driven Void *Collapse*

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Recent advances in inertial confinement fusion (ICF), including experiments at the National Ignition Facility demonstrating scientific breakeven, highlight the need to characterize the hydrodynamics of ICF capsule materials during shock compression [1–7]. Achieving higher fusion yields requires characterization of the ablator under shocks, as defects such as voids disrupt compression symmetry and seed instabilities that degrade implosion performance. Direct observation of these processes is therefore important for validating hydrodynamic models used in ICF target design. Here we use single-shot, x-ray phase-contrast imaging to study shock-driven void collapse in ICF-relevant materials under high-energy-density conditions. Experiments were performed at the Matter in Extreme Conditions (MEC) instrument at the Linac Coherent Light Source (LCLS), where targets containing hollow SiO2 void spheres embedded in SU8 were driven by a long-pulse laser to generate shock compression. Femtosecond two-dimensional XPC images were recorded at multiple x-ray delay times, producing a sequence capturing the evolution of void deformation and collapse as the shock propagates through the material. Since single-pulse XFEL measurements exhibit shot-to-shot beam fluctuations and detector/lens nonuniformities, the images were processed using flat-field correction combining image registration [8–11] and principal component analysis (PCA) [8,10,12]. Quantitative phase retrieval was then performed using complementary algorithms, including a contrast transfer function method solved with fast alternating direction method of multipliers (CTF-fADMM) [13–15] and a projected gradient descent (PGD) approach [16,17], enabling reconstruction of projected electron-density and areal-density maps. The reconstructed density maps are compared with synthetic XPC images from radiation-hydrodynamic simulations using the xRAGE code. These comparisons reveal the morphology and evolution of void collapse while highlighting similarities and discrepancies between modeled and experimentally observed density maps. The results demonstrate the capability of single-shot XPC imaging to resolve shock-driven processes and provide possible experimental constraints for improving hydrodynamic models of defect-driven instabilities in ICF-relevant materials.

Tracking Strain Evolution and Defect Dynamics in Platinum Nanocrystals Under High Pressure Using Bragg Coherent X-ray Diffraction Imaging

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Crystal defects play a central role in governing the mechanical and functional behavior of materials[1–5], yet their collective organization, stability, and transitions under external stress remain difficult to access experimentally at the nanoscale. Here, we investigate the evolution of defect configurations in a single crystalline platinum nanoparticle supported on a yttria-stabilized zirconia (YSZ) substrate, using in situ high-energy Bragg Coherent X-ray Diffraction Imaging (BCDI) during compression in a diamond-anvil cell[6–7].

BCDI provides three-dimensional access to displacement and strain fields with nanometric spatial resolution and high strain sensitivity, enabling direct visualization of line defects and dislocation loops. At low applied pressure, the Pt nanocrystal is largely defect-free, except for a single, well-defined dislocation line located at the particle–substrate interface, which remains stable up to approximately 2.7 GPa. Upon increasing pressure beyond a critical threshold of about 5 GPa, a sharp transition occurs, characterized by the collective nucleation of multiple dislocation lines and loops throughout the particle volume, accompanied by strong distortions of the coherent diffraction pattern.

Time-resolved measurements at constant pressure reveal partial relaxation of the defect population, while pressure cycling demonstrates a striking reversibility: upon unloading, the nanocrystal recovers its initial defect state with the same interfacial dislocation line at the identical location. Subsequent recompression reproducibly regenerates the same defect configurations and dynamics, including loop formation and glide.

These observations provide direct experimental evidence that plastic activity in supported nanocrystals can be understood in terms of stress-driven transitions between distinct, reproducible defect configurations. Such configurations can be viewed as defect phases, defined by their topology, spatial organization, and stability, whose transitions are controlled by external thermodynamic loading and internal stress fields. This work highlights the potential of coherent X-ray imaging to experimentally resolve defect phase transitions and to inform defect-phase-based strategies for materials design.

X-ray Coherent Surface Scattering Imaging for Critical-Dimension Metrology in Reflection Geometry

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Extreme ultraviolet (EUV) lithography for producing nanoelectronics with sub-10 nm nodes brought about ultrahigh-precision optics and masks. The process is based on EUV propagation and manipulation in reflective optical paths, creating challenges in the fabrication and metrology of the elements. Metrology tools with even higher resolution and precision are needed in the pipeline of manufacturing steps to ensure quality, reliability, performance, and yield. Unprecedented challenges are emerging in the metrology of critical dimensions (CDs), such as line 3D profile, roughness, and defects, at a few nanometers (nm) or even sub-nm precisions in the reflective multiplayer optics and masks with minimal preparation. Conventional optical scatterometry is fundamentally wavelength-limited, while electron-beam methods are surface-weighted, dose-sensitive, and rely on model-dependent reconstructions to infer buried or sidewall information. Hard X-rays provide a complementary approach, as their short wavelengths and tunable penetration enable dimensional probes of surfaces and near-surface stacks in reflection geometry, aligning naturally with EUV mask and wafer metrology. New hard X-ray CD metrology in reflection geometry—where X-rays are reflected from the patterned wafer and encode 3D structure in the reflected field—requires minimal sample preparation and is nondestructive. We present the reflection-geometry CD metrology capabilities newly commissioned at the CSSI (Coherent Surface Scattering Imaging) beamline 9-ID of the Advanced Photon Source (APS), Argonne National Laboratory. Benefiting from the recent APS Upgrade, the coherent flux has increased significantly, critical for CSSI with a much-improved signal-to-noise ratio. The metrology uses phase-sensitive reconstructions of aperiodic patterns. We also developed a reflection-geometry X-ray interferometry/holography mode that exploits interference between the sample-scattered field and its reflection from the substrate (a Lloyd’s-mirror-like geometry). Operating off-specular (dark-field) yields high-contrast speckle patterns exquisitely sensitive to out-of-plane morphology, enabling single-view 3D inference on planar patterns supported by thick, optically flat substrates with nm and even sub-nm resolution.

Nanoscale Ultrafast Lattice Modulation with Hard X-ray Free Electron Laser

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Ultrafast optical laser-based techniques have enabled the probing of atomistic processes at their intrinsic temporal scales with femto- and attosecond resolution. However, the long wavelengths of optical lasers have prevented their interrogation and manipulation with nanoscale spatial specificity. Advances in hard X-ray free-electron lasers have enabled progress in developing X-ray transient-grating spectroscopy, a technique that aims to coherently control elementary excitations with nanoscale X-ray standing waves. Thus far, the realization of this technique at the nanoscale has been a challenge. Here we demonstrate X-ray transient-grating spectroscopy with spatial periods of the order of 10 nm via the subfemtosecond synchronization of two hard X-ray pump pulses at a precisely controlled crossing angle. This creates a thermal grating and preferentially excites coherent longitudinal acoustic phonon modes with the transient-grating wavevector. On probing with a third, variably delayed, X-ray pulse with the same photon energy, time-and-wavevector-resolved measurements of the modulation of the induced scattering intensity provide evidence of ballistic thermal transport at nanometre scales. These results highlight the potential of X-ray transient gratings as a powerful platform for studying nanoscale transport in condensed matter and the coherent control of nanoscale dynamics.

Uncovering the dynamical modes in chiral spin/polar textures through dynamical phase-field simulation and X-ray diffraction pattern calculation.

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Understanding the dynamical modes of complex magnetic and polar textures is essential for advancing functional materials based on topological excitations and coupled order parameters. In systems such as Skyrmion-hosting magnetic heterostructures and ferroelectric superlattices, collective excitations of spin and polarization dynamics can be achieved by acoustic probe methods, through magnetoelastic or electrostrictive coupling effects. However, resolving the full spectrum of these modes in these complex heterostructures remains a theoretical challenge.

Here, we present a theoretical framework for resolving the collective excitation spectrum of complex magnetic and polar textures under acoustic driving, by incorporating dynamical phase-field simulation methods and time-dependent X-ray diffraction (XRD) analysis. Our phase-field simulation approach enables selective excitation of dynamical modes via broadband or frequency-tunable strain pulses, providing access to both localized and propagating dynamics in heterogeneous systems. Unlike conventional linearized approaches, this method captures the full spatial complexity of the textures and their nonlinear coupling to lattice degrees of freedom. A key advance of this work is the direct computation of time-dependent XRD signals from simulated polarization and displacement fields. Building on atomistic reconstruction of scattering amplitudes from phase-field outputs, we obtain time-resolved diffraction intensity and its frequency-domain spectrum. This enables a direct bridge between mesoscale simulations and coherent scattering experiments, such as time-resolved coherent diffraction imaging and photon correlation spectroscopy.

As representative examples, we consider (i) ferroelectric vortex arrays in $PbTiO_3/SrTiO_3$ superlattices, where acoustic excitation couples to polarization rotation and domain wall dynamics, producing characteristic satellite evolution in reciprocal space, and (ii) Skyrmion-hosting Fe_3GaTe_2 membranes, where magnetoelastic coupling enables acoustic excitation of Skyrmion collective modes and spin-acoustic wave hybridization.

This work establishes a pathway for integrating dynamical phase-field simulations with coherent scattering techniques, enabling quantitative comparison between theoretical simulation and coherent experiment measurables for complex magnetic and ferroelectric heterostructures.

Single-Frame Coherent X-ray Imaging of Extended Objects Using Randomized Zone Plates

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The advent of upgraded diffraction-limited light sources offers unprecedented coherent flux, accelerating the adoption of coherent diffraction imaging techniques, such as X-ray ptychography, for nanoscale characterization in scientific discovery. Fully realizing the potential of these techniques also requires advanced beam conditioning; previous studies indicate that optimizing the illumination profile is essential for enhancing both image quality and experimental throughput [1, 2]. Building on this, we leverage highly optimized randomized zone plates [3] to generate a structured, randomized probe. We demonstrate that this tailored illumination not only yields superior imaging quality but also drastically increases throughput by relaxing the traditional requirement for densely overlapping on scan spots. Critically, we report the successful implementation of single-frame coherent imaging [4] utilizing this structured probe at the upgraded Advanced Photon Source (APS-U): a quantitative real-space image of an extended object can be reconstructed from a single diffraction pattern. By eliminating the mechanical scanning bottleneck, this approach can push temporal resolution directly into the sub-millisecond regime, limited solely by the frame rate of modern X-ray pixel array detectors. When combined with a pump-probe scheme, the accessible timescale can be further extended to the X-ray pulse duration [5]. Ultimately, this scan-free capability establishes a powerful new framework for visualizing and tracking structural dynamics in complex material systems with simultaneous high spatial and temporal resolution.

Poster Presentation #70

Dose efficient X-ray computed Tomography enabled by randomized zone plate

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Advances in X-ray source brilliance have driven major breakthroughs in coherent X-ray imaging. Ptychographic X-ray computed tomography (PXCT) enables non-destructive three-dimensional imaging with nanometer scale resolution benefiting from the high coherence and flux provided by modern X-ray facilities, achieving state-of-art resolutions down to 4 nm in integrated circuits. However, the continuous increase in source brilliance also introduces substantial challenges, including enhanced radiation damage, photon-counting detector saturation, and increasing ratio of scanning overhead to exposure time that ultimately limits further acceleration of data acquisition.

In this ongoing work, we investigate randomized probe imaging (RPI) tomography as a fast and dose-efficient alternative for three-dimensional coherent X-ray imaging. A randomized zone plate (RZP), incorporating intentionally introduced phase aberrations, generates a focal spot with a fine, spatially uniform speckle texture. This fine speckle structure probe encodes high spatial frequency information of the sample and allows the use of substantially larger ptychographic scan step, thereby reducing the total number of exposures required for a given field of view.

Most importantly, the speckle-rich structured illumination enables single-shot imaging via RPI. When combined with tomographic rotation, additional angular diversity will stabilize the iterations, allowing the achievable resolution to approach that of ptychographic tomography at an equivalent radiation dose.

We aim to establish a joint RPI–tomography framework for rapid, high-resolution volumetric imaging. The method will be evaluated for both isolated specimens smaller than the beam waist and extended samples using internal tomography. Our goal is to achieve resolution comparable to PXCT while significantly reducing acquisition time and radiation dose under identical experimental conditions.

Ptychography-Constrained Dynamic Coherent Diffraction Imaging for Nanoscale Operando Electrochemical Processes

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Dynamic electrochemical processes evolve at nanometer length scales but often occur on timescales that are difficult to capture with conventional scanning X-ray microscopy. Ptychography can provide high-resolution structural information, but its scanning-based acquisition limits its application to rapidly evolving systems. In contrast, coherent diffraction imaging (CDI) is a single-shot lensless imaging technique that is better suited for tracking transient nanoscale processes with high temporal resolution. However, CDI phase retrieval is often ill-posed because of the lack of sufficient spatial constraints. Here, we overcome this limitation by incorporating prior structural information obtained from ptychography measurements acquired before and after the dynamic CDI experiment. These ptychography reconstructions provide physically meaningful constraints that stabilize phase retrieval and enable nanoscale imaging of dynamic CDI data with high temporal resolution. Using copper pulse-reversal electrodeposition (Cu PR-ED) in an operando liquid electrochemical cell as a model system, this framework allows us to follow the evolution of electrochemically deposited Cu particles in real time and establishes a practical strategy for bridging the spatial-resolution advantage of ptychography with the temporal-resolution advantage of CDI.

Rheo-XPCS study of microstructural and rheological training and memory of nanocolloidal soft glasses under cyclic shear

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An intrinsic feature of disordered and out-of-equilibrium materials, such as glasses, is the dependence of their properties on their history. An important example is rheological memory, in which disordered solids obtain properties based on their deformation history. We employ x-ray photon correlation spectroscopy (XPCS) with in situ rheometry to characterize memory formation in a nanocolloidal soft glass due to cyclic shear [1]. During a cycle, particles undergo irreversible displacements composed of a combination of shear-induced diffusion and heterogeneous strain fields. At lower shear amplitudes, the displacements resemble a random walk in which the directions in each cycle are independent of those in preceding cycles, while at high amplitude the irreversible displacements in consecutive cycles become correlated. The magnitudes of the displacements decrease with each cycle before reaching a steady state where the microstructure has been trained to achieve enhanced reversibility. At amplitudes below and near yielding, these decreases are monotonic, while well above yielding they are nonmonotonic, suggesting evidence of shear banding. Accompanying this microstructural training are corresponding decreases in the dissipation during each cycle and the magnitude of the residual stress towards steady-state values. Memory of the training is revealed by measurements in which the amplitude of the shear is changed after steady state is reached. The magnitude of the particle displacements as well as the dissipation and the change in residual stress vary nonmonotonically with the new shear amplitude, having minima near the training amplitude, thereby revealing correlated microscopic and macroscopic signatures of memory.

Poster Presentation #73

Multislice coherent x-ray imaging beyond depth of focus limits for neurobiology

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Hard X rays offer fundamental advantages for the imaging of circuitry in neurobiology: they offer short wavelengths with the potential for 10-20 nm spatial resolution for synapse identification, and the ability to penetrate millimeters into tissue so as to reduce or avoid tissue sectioning. With modern coherent x-ray sources, the imaging time can be reduced to tractable values [1]. However, to fully realize this potential, one must image volumes beyond the conventional depth of focus limit of DOF=5.4δr2/λ, where δr is the transverse spatial resolution and λ is the x-ray wavelength. One approach that has been demonstrated in simulations [2,3] is the use of multislice methods for wavefield propagation, where successive steps of optical modulation and Fresnel wave propagation are used to describe coherent wave propagation through a thick object computationally divided into thin slabs. For a present guess of a 3D refractive index distribution n(r), one can then predict the intensity recorded at each of many rotation angles θ, and thus arrive at predicted I[θ,n(r)]. One can then use numerical optimization methods to adjust n(r) and thus minimize the difference between predicted I[θ,n(r)] and measured I[θ]. We describe first experiments to collect experimental data to test this approach for the imaging of mouse olfactory bulb, and initial efforts towards image reconstruction of continuous objects beyond the depth-of-focus limit.

Poster Presentation #74

Operando Coherent X-ray Imaging of Copper Electrodeposition Nucleation and Growth Dynamics

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Advances in synchrotron light sources now allow researchers to watch electrochemical reactions unfold in real time at the nanoscale. However, systems like copper electrodeposition (Cu ED) are sensitive to X-ray radiation — high photon flux can trigger unwanted side reactions, including beam-driven copper deposition and breakdown of the surrounding electrolyte. These beam-induced effects can distort nucleation and growth behavior, making it difficult to extract reliable information about the true electrochemical process.

In this work, carried out at the Hard X-ray Nanoprobe (HXN) beamline at NSLS-II, we use two X-ray imaging methods to study Cu ED dynamics while keeping radiation damage to a minimum by using beam attenuators and shorter exposure time. Quasi-in-situ ptychography captures how copper particles nucleate and grow when pulse reverse current is applied intermittently, delivering high-resolution images of the deposit structure at key stages with low cumulative X-ray dose. Operando coherent diffractive imaging (CDI) tracks fast particle changes at 5 ms time interval, revealing dynamic behavior that would otherwise be missed. Avrami modeling and power-law growth analysis show that beam exposure speeds up deposition kinetics without changing the underlying growth mechanism. We find that the observation mode—continuous (in- situ) versus intermittent (quasi-in-situ)—significantly influences deposition behavior, resulting in distinct particle growth power-law dynamics. These results shed light on how current waveform design controls deposit microstructure, with practical implications for copper deposition in semiconductor devices, electrocatalyst fabrication, and battery electrode engineering.

Nanoscale Imaging of Framework Flexibility and Molecular Accessibility in Zeolite Catalyst by Bragg Coherent Diffraction Imaging

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Zeolites are widely used as catalysts. Their performance relies on molecular transport through their microporous framework. Framework deformations, known as zeolite ‘flexibility’, play a critical role in regulating adsorption, diffusion and catalytic selectivity. Catalytic performance can be impacted by modification of pore apertures, connectivity and diffusion pathways; properties linked to this flexibility. Minor pore aperture changes have been shown to drastically improve separation performance in ITQ-55 type¹, while some frameworks can undergo unit cell volume variations of up to 20%². However, direct experimental observation of such nanoscale framework responses under reaction remains extremely limited.
We employed Bragg coherent X-ray diffraction (BCDI) to directly visualise lattice dynamics in individual ZSM-5 zeolite crystals during ethanol dehydration catalysis. Molecular adsorption and diffusion changes were tracked in single ZSM-5 crystals by reconstructing the three-dimensional strain distribution to understand how the framework responds to changing reaction environments.

I will show how our results provided direct nanoscale evidence that zeolite flexibility is dynamically modulated during catalysis, influencing molecular accessibility and diffusion pathways³. This work also demonstrates the capability of BCDI to probe structure-function relationships in nanoporous catalysts under in situ conditions.

Spectroscopic Bragg Coherent Diffraction Imaging of Single Nanoparticles

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Characterizing nanoscale displacement fields, compositional variations, and defects in heterogeneous catalysts remains a central challenge in materials science and energy-conversion research. Bragg Coherent Diffraction Imaging (BCDI) [1] can deliver three-dimensional strain maps with ~10 nm resolution, yet chemical inhomogeneities often blur the distinction between strain and compositional contributions. This is an especially acute issue for chemically heterogeneous structures such as NiFe and PtPd, climate-critical alloyed bimetallic catalysts used in CO_2 hydrogenation. In these systems, compositional and structural changes under reaction conditions are coupled yet poorly resolved by existing techniques.

We have developed a nano-focused 3D spectroscopic Bragg coherent imaging technique at the nanoprobe ID01-EBS beamline of The European Synchrotron (ESRF). By combining BCDI with Multiwavelength Anomalous Diffraction (MAD), spectro-BCDI reveals both chemical (composition, oxidation states and bond structure) and structural (morphology, lattice strain and defects) information about nanocatalysts. Nano-focused fluorescence spectroscopy is applied alongside [2].

This talk presents the technique through simulated diffraction data with realistic photon statistics, from which we validate accurate composition recovery across the reconstructed volume. We then show experimental results from two systems: NiFe nanocrystals at the Ni K-edge (8.333 keV) and PtPd nanoparticles at the Pt L3-edge (11.564 keV). The two systems probe the technique under substantially different experimental conditions in terms of fluorescence background, edge morphology, and available anomalous contrast. Future work will apply spectro-BCDI under in-situ gas conditions to track how composition and strain evolve in individual nanocrystals during CO_2 hydrogenation, directly linking atomic-scale structure to catalytic selectivity.

Escaping the Permittivity-Mobility Trap: A Route to High Permittivity in Dipolar Polymer Melts

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Despite transformative potential, large dielectric constants in polymers remain elusive due to a key trade-off: dipoles simultaneously increase polarizability and the glass transition temperature (Tg). Once Tg exceeds the operating temperature, dipole mobility is frozen and dipole relaxation is suppressed, dramatically decreasing permittivity. This establishes a limit on the dielectric constant in dipolar polymers that we term the “permittivity–mobility trap” (PMT). The PMT is particularly prominent for polyzwitterions, whose dense Coulombic and dipole interactions cause phase separation and high thermal transition temperatures even at modest (10–20 mol%) incorporation ratios. We present a polysiloxane that breaks this trend, with a glass transition temperature of –14 °C despite 91 mol% pendant zwitterions. Moreover, it features a static dielectric constant of 420 at 298 K, the largest, to our knowledge, reported for a pure polymer to date. We attribute its low Tg and large dielectric constant to the long and flexible inter-charge spacers in each zwitterionic repeat unit, which simultaneously dilute strong interactions and increase dipole moment. This design paradigm, comprising few dipoles with large moments, offers a strategy to amplify the dielectric constant in soft materials. Yet, its structure and polarization behavior in electric fields is not well understood. We anticipate that X-ray scattering in AC electric fields offers a unique opportunity to quantitatively map the field- and time-dependent structure of soft zwitterionic materials.

On Orbital Angular Momentum–Dependent Coherent Bragg Diffraction Imaging

Prof Edwin Fohtung[1], *Dmitry Karpov[2], Ewen Bellec[2], Nimish Narzirkar[1], Jackson Andersen[1], Oji Ugwumsinachi[2], Steven Leake[2], Tobias Schülli[2]*
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Structured X-ray beams carrying orbital angular momentum (OAM) provide a new degree of freedom for coherent scattering experiments. Here we investigate how twisted X-ray illumination modifies coherent Bragg diffraction and explore the extension of coherent Bragg diffraction imaging (BCDI) to OAM-resolved measurements. Experiments were performed at the ID01 beamline of the ESRF using a fabricated spiral zone plate to generate X-ray beams with well-defined OAM states.

We studied model systems with distinct structural symmetries, including an achiral Pt nanocrystal, intrinsically chiral Te, and chiral ferroelectric polarization domain textures in a quasi-2D $BaTiO_3$ membrane. Coherent X-ray Bragg diffraction measurements were carried out for multiple OAM modes (ℓ = −3, −1, 0, +1, +3) from small isolated nanocrystals.
The resulting 3D Bragg diffraction intensities exhibit systematic OAM-dependent contrast variation in a helical dichroic mode, indicating that the beam has access to an OAM-resolved scattering form factor arising from higher-order multipole interactions. Such OAM-resolved Bragg electron densities may provide access to new physics, including symmetry-selective scattering, chiral lattice distortions, orbital-current contributions to the structure factor, and other angular-momentum–dependent scattering channels. These results establish a framework for orbital-angular-momentum–dependent coherent Bragg diffraction imaging and highlight the potential of structured X-ray illumination for probing symmetry, chirality, and lattice distortions in complex materials.

New Soft X-ray Nanocale Imaging capabilities at NSLS-II

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Soft X-ray spectromicroscopy provides exceptional chemical sensitivity through near-edge X-ray absorption fine structure (NEXAFS), as well as sensitivity to geometric and magnetic anisotropy via linear and circular dichroism. When combined with nanoscale spatial resolution and coherent imaging approaches, soft X-ray microscopy becomes a powerful tool for probing the structure, chemistry, and functionality of complex materials.

The new Soft X-ray Nanoprobe (SXN) beamline currently under construction at the National Synchrotron Light Source II (NSLS-II) is designed to fully exploit the high brightness and coherence of the NSLS-II source. SXN will deliver world-leading coherent photon flux in the energy range from 250 to 2500 eV with full polarization control, enabling advanced coherent imaging and spectromicroscopy capabilities at the nanoscale. In particular, the beamline will support high-resolution ptychography and other coherent diffraction imaging approaches, providing quantitative phase and amplitude contrast with chemical and magnetic sensitivity.

In this presentation, I will discuss the opportunities and challenges in designing a beamline optimized for coherent soft X-ray nano-imaging, including considerations in coherence preservation, optical design, and instrument stability. I will also introduce the nanoISM endstation and outline how SXN will enable new studies in materials science, energy technologies, microelectronics, quantum materials, and environmental science. Finally, I will provide an overview of the current status and future plans for the SXN beamline.

In situ imaging of materials in nuclear reactor environments

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The accumulation of lattice defects induced by irradiation in structural components of nuclear reactors is fundamental to their dynamical degradation, especially whilst being subjected to corrosive and aqueous environments. The direct observation of radiation-induced defects has so far been limited to electron imaging techniques due to their high resolution and sensitivity to crystalline defects. To further improve the current understanding of how lattice defects can lead to structural damage, it is important to address the evolution of such defects in real time, and in the absence of free surfaces that can affect their behavior. In this study, we present a novel approach to classify and quantify radiation-induced defects in metals, using Bragg Coherent Diffraction Imaging (BCDI), a non-destructive and high resolution imaging technique, that can provide access to the strain tensor within crystalline samples. By using a highly focused synchrotron beam, the probe also acts as a source of radiolysis, locally perturbing the Light Water Reactor Chemistry, and mirroring the effect of neutron induced radiolysis in nuclear reactors. The competing adsorption of beam-induced radicals on specific metallic surfaces observed experimentally is studied by Density Functional Theory, while the defects annihilation is confirmed using discrete dislocation dynamics calculations. Meanwhile, the link between defect mobility and radical insertion is simulated using Molecular Dynamics.

Hydrogen-Driven Phase Transitions in Palladium Nanoparticles Revealed by In Situ BCDI

Petra Khater[1,2,3,4], *Marie-Ingrid Richard*[1,2], *Frederic Maillard*[4], *Tobias Schülli*[1], *Steven Leake*[1], *Ewen Bellec*[1], *Kyle Olson*[1,2,3,4], *Clément Atlan*[1], *Michael Grimes*[1], *Mor Levi*[5], *Eugen Rabkin*[5], *Joël Eymery*[2,3]
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The advent of 4th-generation X-ray light sources offers transformative opportunities for in situ/operando characterization of the structural evolution of nanoparticles in reactive liquid or gas environments. In this presentation, I will illustrate how Bragg coherent X-ray diffraction imaging (BCDI) [1–3] enables direct probing of the strain fields, lattice deformations, and defect dynamics within palladium (Pd) nanocrystals during its hydrogenation. The unique hydrogen (H) absorption properties of Pd underpin its widespread applications in water electrolysis, hydrogenation reaction, hydrogen storage, and hydrogen sensing technologies [4]. However, key questions remain about the mechanisms governing H absorption in Pd crystals, including the nature of the hydride nucleation sites and the dynamics of the H-poor (α) to the H-rich (β) phase transition.

Here, we investigated the interplay between H2 partial pressure and lattice response at room temperature, using in situ BCDI at the ID01 beamline of the ESRF. We resolved strain and lattice parameter distributions with nanometer precision during the α-to-β phase transition, providing insights into H absorption dynamics (Figure 1). We also address open questions on hydride nucleation, including whether it initiates preferentially at structural defects or strained regions, or uniformly across the nanoparticle surface, and whether the α-to-β phase transformation occurs through sharp transitions or two-phase coexistence. This work demonstrates BCDI's ability to visualize structural dynamics in reactive environments, advancing our understanding of phase transformations in Pd systems and paving the way for the optimization of Pd-based materials for use in energy conversion and storage applications.

Advancing Coherent X-Ray Science with High-Speed Detection and Seamless Data Processing

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Coherent X-ray techniques - ptychography, coherent diffraction imaging (CDI), and X-ray photon correlation spectroscopy (XPCS) - place uniquely demanding requirements on detectors: single-photon sensitivity to resolve weak coherent speckle, high dynamic range to capture intense central maxima alongside faint high-q signal, and microsecond-to-millisecond framing to follow fast dynamics and fast scanning speeds. At the same time, the resulting data rates and volumes increasingly bottleneck the experiment rather than the source. Many of these challenges are addressed with photon counting detectors such as the PILATUS4 and EIGER2 [1-4]. Here we present recent developments spanning the relevant energy range and timescales: the charge-integrating JUNGFRAU 4M with 3-level dynamic gain switching for high-flux CDI and serial crystallography; an EIGER2-based LGAD detector extending photon counting into the soft X-ray regime for XMCD ptychography; and the SELUN ASIC enabling 120 kHz XPCS ptychography with on-chip floating-point compression. These are coupled to real-time correction, compression [5, 6, 7], and cloud-based processing pipelines - the DECTRIS CLOUD - to keep data handling from limiting scientific throughput**.**

Combining Dark Field X-ray Microscopy with Coherent Measurements at CHEX beamline

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Dark-field X-ray microscopy (DFXM) is a full-field imaging technique that provides structural contrast by imaging at a selected Bragg diffraction condition. Its X-ray penetration enables studies in complex in situ and in operando environments, while full-field acquisition provides rapid, direct visualization. By choosing the diffraction condition and analysis channel, DFXM can emphasize specific contrast mechanisms (e.g., domains, orientation, or strain), making it well suited for probing surfaces, interfaces, and thin films under operating conditions. Although DFXM is generally faster than scanning-probe approaches, acquisition rates are often limited by photon statistics (typically on the order 0.1∼10 Hz). The APS Upgrade provides substantially increased coherent flux, enabling dynamic studies with X-ray photon correlation spectroscopy (XPCS) on much shorter timescales. A key challenge in thin-film XPCS is connecting measured correlation functions to the underlying domain structure and its evolution. Here we propose a correlative approach: high-speed dynamics from XPCS combined with intermittent DFXM “snapshots” of domain configurations, integrated through AI-assisted analysis to link structure and dynamics.

We will discuss the feasibility and potential of this capability in studying, for example, micro-electronic devices, at the Coherent High-Energy X-ray (CHEX) beamline at the Advanced Photon Source.

Poster Presentation #84

Spatially Resolved Thin-Film Thickness Mapping via Coherent Grazing-Incidence Diffraction Imaging with Parratt Regularization

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Conventional specular reflectometry yields angle-dependent reflectivity averaged over the illuminated footprint, providing no lateral spatial resolution. We present a computational framework for spatially resolved thin-film thickness and roughness mapping from grazing-incidence coherent diffraction data collected across multiple incident angles. A geometry-aware multislice forward model maps a 2D thickness distribution to angle-dependent diffraction predictions, with a physics-informed Parratt reflectivity penalty regularizing the otherwise ill-posed inversion. Probe and thickness updates are decoupled, with each variable updated via a gradient-based scheme appropriate to its structure. The pipeline is GPU-accelerated and parallelized across multiple devices. We evaluate the approach on simulated grazing-incidence datasets from a patterned Au-on-Si phantom and experimental data, examining convergence behavior and the stabilizing role of the reflectivity constraint. This work establishes a physically grounded pathway toward pixelwise surface reflectometry at coherent synchrotron sources.

Imaging Surface Topography using Coherent X-ray Reflectivity: Formalism, Simulations and Initial Results*

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A formalism for understanding coherent X-ray reflectivity (CXR) from the surface of a semi-infinite crystal having an arbitrary height profile, h(x,y), is presented [1]. These results consider interfacial images that would be obtained from phasing and inversion of coherent specular X-ray reflectivity data measured in a “rocking scan” at a vertical momentum transfer, Qz0, with a vertical range, ΔQz. The formalism predicts that the interface appears as a complex “effective density” whose amplitude has a maximum at the surface height at each position within the surface plane, and with a vertical width that is defined by the vertical resolution, ~2π/ ΔQz. The phase of the effective density has two contributions: a vertical phase gradient that incorporates the details of the interfacial structure and specific choice of measurement conditions, and a phase pre-factor that is controlled by the surface height. This understanding enables direct observation of nanometer-scale interfacial topography, with Å-scale sensitivity to surface heights, and is directly analogous to the sensitivity of Bragg Coherent Diffraction Imaging to sub-nm lattice displacements. These results suggest that CXR can be thought of as a form of dark field imaging with respect to the bright field BCDI approach, and as a form of super-resolution imaging for interfacial topography.

Precipitation-induced strain field in Ni-based superalloys imaged by Bragg Projection Ptychography

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Understanding and quantifying local strain fields in Ni-based superalloys is critical for elucidating degradation mechanisms that limit their structural integrity at elevated temperatures. In these alloys, lattice parameter mismatch between the γ-matrix and coherent γ′-precipitates generates internal stresses that can promote crack initiation through strain-age cracking during thermal exposure. Direct nanoscale characterisation of these strain fields is therefore essential for establishing microstructure–property relationships and improving alloy design. In this work, we investigate the strain field associated with embedded γ′-precipitates within the γ-matrix of two Haynes 282 Ni-based superalloys from addictive manufacturing and wrought processing. Scanning transmission X-ray diffraction (STXRD) with a focused beam size of 60 × 60 nm² was employed to spatially resolve diffraction from the ⟨200⟩ and ⟨100⟩ reflections. Overlapping scanning steps allowed sufficient conditions for Bragg Projection Ptychography (BPP) to be employed, mapping the local strain variations with phase retrieval. Using X-ray fluorescence signal, the strain features and γ′-precipitates position were correlated, indicating that the strain variations were indeed occurring in the vicinity of individual precipitates. The results show measurable differences in the strain field between the two samples, providing direct insight into the elastic interaction between the two phases at the nanoscale, opening new opportunities for employing STXRD, BPP or analogue techniques such as Bragg CDI and Bragg Ptychography to explore the evolution of strain fields in Ni-based superalloys.

Anomalous Atomic Relaxation in high-Tc Superconductors

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High-temperature superconductivity in cuprates is deeply connected to the underlying atomic lattice. This has been demonstrated by the observation of electronic stripes and patchy states whose properties are strongly correlated with local structural heterogeneity [1–3]. However, the temporal stability of the lattice itself remains largely unexplored, even though it may determine the ultimate lifetime of intertwined electronic structures. We will present our recent X-ray Photon Correlation Spectroscopy (XPCS) studies on the quasi-static atomic relaxation dynamics in two classes of cuprate superconductors: La2-xSrxCuO4 and YBa2Cu3O6+y [4–6]. Upon cooling, we find pronounced relaxational anomalies coincident with the onset of charge-density-wave order and superconductivity. Our results point to a strong coupling between atomic relaxation and electronic states, and suggest that this interplay may be a pervasive feature across the cuprate family.

Resolving Coupled Lattice and Magnetic Dynamics in $Gd_3Fe_5O_{12}$ with Time-Resolved Resonant X-ray Diffraction

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Understanding the interaction between lattice and spin degrees of freedom on ultrafast time scales in magnetic insulators is essential to uncover the fundamentals of magnetic transport phenomena and advancing spintronics, magnonic, and spincaloritronic technologies. Wavevector-resolved acoustic strain induced magnetization and magnetic dynamics in the ferrimagnetic Gadolinium Iron Garnet, $Gd_3Fe_5O_{12}$, are investigated using femtosecond time-resolved resonant magnetic x-ray diffraction. The optical pulse on Pt transducer launches longitudinal acoustic strain pulse that propagates into the GdIG layer. By tuning X-ray energy to Gd L2 resonance, lattice and magnetic responses are probed independently. The longitudinal acoustic pulse modulates magnetism through the inverse magnetostriction and generates coherent magnetic oscillations in picosecond timescales. The structural dynamics reveal a distinct acoustic mode near 0.19 THz across all measured wavevectors, consisted with the repeated Pt excitation. In addition, dispersive longitudinal acoustic phonons are observed at higher frequencies and varying wave vectors. The magnetic resonance measurement reveals multiple magnetic oscillations over a wide range of wave vectors. Some magnetic oscillations coincide with the 0.19 THz acoustic resonance, and others with the dispersive longitudinal acoustic phonons, providing direct evidence of coherent interaction of magnetism and lattice strain. An additional magnetic oscillation near 0.46-0.5 THz at all measured wave vector may be associated with a Gd precessional mode. These results motivates for future time resolved x-ray microscopy studies, including coherent diffraction imaging and ptychography to directly resolve nanoscale strain fields, magnetic domains and their response to ultrafast acoustic pulse.

In Situ Nanodiffraction of SiC for Real-Time Polytypic Control

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We sketch out the plans and recent work towards integrating a metal oxide chemical vapor deposition (MOCVD) machine into the CHEX beamline at the newly upgraded APS for the purpose of silicon carbide (SiC) growth and in situ characterization. SiC has tremendous potential for wafer-scale quantum information science (QIS). SiC has over 250 polytypes, or stacking arrangements, offering possible avenues for control of the environment around the defects typically used as qubits. However, there are well-documented issues in achieving suitably low defect SiC necessary for quantum computing, and control of heteropolytypes is absent. Synthesis of pure single-polytype SiC, as well as low-defect heteropolytypic SiC structures will allow for improved defect coherence as well as greater qubit control. In situ single crystal x-ray diffraction allows us to monitor these phases as they evolve and form, allowing us to determine what specific MOCVD conditions quantify the polytypic phase boundary. Our team has succeeded in preliminary in situ monitoring of Bragg peaks on crystal truncation rods which indicate specific SiC polytypes, showing heteropolytism. Additionally, with the upgraded coherence of the APS, we will be able to recover x-ray phase information from our sample, helping us identify the different polytypes' grain boundaries. We will design and execute surface diffraction experiments to systematically uncover these polytypic phase space regimes. We plan to begin our exploration by attempting a 4H homopolytypic growth, and then exploring an intentional 4H-3C-4H heterostructure that can be used to make membranes. Additionally, we plan to harness this increased coherence to perform XPCS measurements of island formation during these growth and processing procedures, gaining more insight into the fundamentals of different polytype formations. We will also be attempting to selectively etch these heteropolytypic structures, in order to make SiC membranes similar to our group's process established in diamond, allowing for tunable and transferabe SiC QIS interfaces.

Ultrafast Above-Bandgap Excitation of Polar Skyrmion Dynamics in PbTiO3/SrTiO3 Superlattices

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Polar Skyrmions arise in ferroelectric/dielectric epitaxial complex oxide superlattices due to the competition between energies associated with the polarization, lattice distortion, and crystallographic texture. The Skyrmions exhibit continuous polarization complex curvatures, forming nanoscale dipolar textures that are topologically distinct from conventional ferroelectric domains. Their stability and reversibility make them promising for ultrafast functional control of controlling nanoscale polarization states that could be exploited for reconfigurable ferroelectric functionality.

Electric-field-induced switching and structural tuning of polar Skyrmions have been explored previously. The transient structural response of the polar Skyrmions following optical excitation above the bandgap is not well understood, specifically in the first few picoseconds after photoexcitation. Here we investigate ultrafast structural dynamics in ferroelectric PbTiO3/dielectric SrTiO3 superlattices using time-resolved X-ray diffraction at Pohang Accelerator Laboratory X-Ray Scattering and Spectroscopy (XSS) beamline. The superlattice thin film was excited using 50 fs-duration pulses with a wavelength of 266 nm. The evolution of the structure was probed using thin film x-ray diffraction and diffuse scattering with an X-ray photon energy of 9.4 keV.

The high brilliance of the coherent XFEL pulses enables the measurements of weak reciprocal space features including diffuse scattering peaks where structural distortions are associated with polar Skyrmion ordering. Following optical excitation, changes in the diffracted intensity arise from transient lattice dynamics. Frequency components observed extend into the THz range, with a notable 0.4 THz frequency we attribute to polar Skyrmion dynamics. Complementary phase-field simulations connect the observed intensity oscillations with Skyrmion dynamics. The simulation and experiment are consistent with a model in which carrier induced screening drives dynamic reconfiguration of polar Skyrmions. This work provides a framework for understanding how optically generated structural changes perturb topological polarization textures on ultrafast timescales.

Ultrafast Visualization of Heterogeneous Strain in Single Palladium Nanocrystals using Coherent X-rays

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The advent of X-ray free-electron lasers (XFELs) has enabled the visualization of structural dynamics at the nanoscale with unprecedented temporal resolution. Here, we exploit the full coherence of an XFEL to investigate the ultrafast heat transfer mechanisms within individual palladium (Pd) nanocrystals, a material of high interest for catalysis. Using an optical laser pump and coherent X-ray diffraction probe, we captured the evolution of single 111 Bragg peaks from individual nanocrystals as a function of delay time and laser fluence. Above a threshold fluence, we observe a striking peak splitting at approximately 30 picoseconds delay, indicating a transient, highly heterogeneous strain state. By forward-modelling the coherent diffraction data, we reconstructed the real-space displacement and strain fields, revealing a sharp strain wave propagating through the crystal. This creates a boundary between an expanded region near the illuminated surface and a compressed region in the crystal interior. The heterogeneous state persists for ~20 picoseconds before thermal equilibration occurs. This behavior contrasts with previous studies on gold nanocrystals, which we attribute to palladium's shorter hot-electron mean free path and higher electron-phonon coupling constant. Our work demonstrates the power of exploiting X-ray coherence to directly image the birth and evolution of nanoscale strain fields during ultrafast heat transfer, providing crucial insights for optimizing energy dissipation in photo-catalytic and plasmonic applications.

Characterizing phase contrast in full-field tomographic imaging at ForMAX

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Propagation-based X-ray phase contrast imaging enables visualization of weakly absorbing materials when highly coherent X-ray beams are available. However, retrieving both absorption and phase shift from a single in-line phase contrast image remains a nonlinear and ill-posed inverse problem. In this work, we apply a nonlinear primal–dual hybrid gradient (NL-PDHG) [1], [2] phase retrieval framework to tomography data acquired at the high-coherence ForMAX beamline at MAX IV, a fourth-generation synchrotron facility.

We assume that an object is defined by its 3D complex refractive index by n, where n is

$$n(x, y, z) = 1 - \delta(x, y, z) + i\beta(x, y, z)$$

where $\delta(x, y, z)$ is the decrement in 3D refractive index and $\beta(x, y, z)$ is the 3D absorption index in Euclidean space.

Using single-distance propagation-based phase contrast images recorded under highly coherent illumination, the NL-PDHG algorithm was used to jointly reconstruct projected absorption and phase shift. The method incorporates the nonlinear Fresnel propagation model and allows separate total variation regularization of absorption and phase [3], while minimising residual between forward projected and intensity images.
Experimental results show stable phase retrieval with minimal artifacts. The nonlinear approach also improved the normalized mean squared error compared with its linearized version. Although multiple regularisation parameters must be selected, the approach resolves internal structures in weakly absorbing, multiphase materials from single-distance measurements, demonstrating the potential of combining high-coherence synchrotron sources with nonlinear regularized phase retrieval methods.

Single Shot Coherent Modulation Imaging and Wavefront Sensing at Free Electron Lasers

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Coherent diffraction imaging (CDI) provides diffraction-limited images of nano-scale samples, making it an ideal technique for time-resolved applications at X-ray free-electron lasers (FELs). However, conventional CDI struggles to reliably image and wavefront-sense extended samples and wavefields without defined support using only a single diffraction pattern. Coherent modulation imaging (CMI) alleviates this problem by introducing a randomly structured modulator near the sample or the focusing optics. This results in a quasi-random speckle pattern at the detector, simultaneously reducing the required dynamic range and introducing additional constraints into the reconstruction process, enabling robust, high-resolution imaging from a single shot. While first demonstrated at synchrotrons, CMI is now being integrated into FEL facilities across various experimental geometries.

In this work, we present several improvements to the CMI scheme utilizing near-field modulation and report results from imaging and wavefront-sensing experiments performed at EuXFEL and PAL-XFEL. We demonstrate the versatility of this approach in both forward- and Bragg-diffraction geometries. Furthermore, we introduce an enhanced reconstruction algorithm that significantly relaxes previous constraints on modulator randomness and the spatial frequency separation between the modulator and the sample. These developments simplify modulator design and broaden the applicability of CMI for high-fidelity, single-shot imaging and wavefront sensing at FELs.

Ultrafast Coherent Diffraction Imaging of Self-Assembled 1 nm Gold Nanoclusters at LCLS

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Self-assembly of gold nanoclusters produces nano- to mesoscale structures with enhanced optical and electronic properties, making them promising building blocks for functional nanomaterials and plasmonic devices. These properties are commonly investigated using spectroscopic techniques, which typically provide only indirect information about the underlying structure. Directly characterizing the structural organization of such assemblies at the nanoscale therefore remains challenging.

Here we recorded single-shot coherent diffraction images at the Coherent X-ray Imaging (CXI) endstation of the Linac Coherent Light Source (LCLS) using intense, few-femtosecond X-ray pulses to investigate assemblies of 1 nm gold nanoclusters.

The recorded diffraction patterns reveal signatures of ordered arrangements within the nanocluster assemblies, extending from hundreds of nanometers up to several hundred micrometers. Such length scales are difficult to access with conventional techniques such as TEM or synchrotron SAXS/WAXS, which are limited by sample thickness, field of view, and scattering contrast. Numerical simulations reproduce the observed scattering features and provide additional insight into the structural organization within the assemblies. Our results demonstrate the capability of ultrafast coherent diffraction imaging to probe the structure of self-assembled nanocluster materials and pave the way for time-resolved studies of dynamic self-assembly processes.

Time-resolved spectroscopy of collective modes in Pb(Mg1/3Nb2/3)0.68Ti0.32O3 using coherent x-ray scattering

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Relaxor ferroelectrics are a well-known but poorly understood class of functional materials in which the electromagnetic response functions are renormalized by the presence of nanoscale heterogeneity in the ground-state polarization texture. Despite decades of research, however, the low-energy excitations associated with this phase have yet to be fully characterized, and the origin of the observed dynamical behavior remains ambiguous. In this work, we use time-resolved coherent x-ray scattering to investigate the low-energy collective modes of a relaxor ferroelectric Pb(Mn1/3Nb2/3)0.68Ti0.32O3 thin film, in which we identify two novel excitations: (1) a 350 m/s surface acoustic wave associated directly with the collective motion of ferroelectric domain boundaries, and (2) a fully localized, non-dispersive collective lattice excitation at a frequency characteristic of an inter-domain interaction. Upon tuning the system away from the relaxor ferroelectric ground state via epitaxial strain, we find that the spectral weight of these excitations is greatly reduced, directly implicating them in the relaxor-like behavior in this material. These findings not only shed new light on the low-energy collective mode spectrum associated with relaxor ferroelectrics, but also represent the first demonstration of "vibrational XPCS," in which the dynamics of a material's mesoscale domain structure may be directly measured in reciprocal space using coherent x-rays.

Experimental model for measuring the spatial coherence of 2D wave fields using phase-space tomography

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Characterizing the spatial coherence of a 2D wave field is essential for understanding the coherent properties of the beam, quantifying partial-coherence effects, and making optimal use of available flux in coherence-based X-ray experiments. We present a practical experimental model for measuring the spatial coherence of 2D wave fields using phase-space tomography. In contrast to more complex implementations, the proposed approach requires only a single cylindrical lens and a series of intensity measurements acquired at multiple propagation distances, making it simple to implement at x-ray beamlines. From these measurements, the 4D coherence function of the wave field can be reconstructed in a direct manner. The method provides an efficient approach to characterize partially coherent beams, which is critical for correcting coherence-induced degradation in imaging and diffraction measurements, improving quantitative interpretation of data, and enabling more effective use of the beam. Because of its simple setup and formulas, this approach offers a practical tool for measuring coherence property of synchrotron x-ray systems.

High-Energy Bragg Coherent Diffraction Imaging for Nanoscale Strain Mapping in Bulk Polycrystalline Ceramics

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Bragg Coherent Diffraction Imaging (BCDI) reconstructs 3D strain fields within isolated crystals at nanoscale resolution and is sufficient to resolve dislocations and extended defects. As defect engineering matures, understanding how localized, heterogeneous strain fields govern bulk material behavior has become an important challenge in materials science. The obstacle is access, BCDI has been historically confined to isolated nanocrystals or surface-adjacent samples, far from the conditions of real engineering materials. Extending these capabilities to micron-sized grains buried inside bulk polycrystals — where grains interact through boundaries and defects couple to mesoscale microstructure — requires both penetrating X-ray energies and sufficient coherence to recover a coherent diffraction signal from deeply embedded grains. Fourth-generation synchrotron sources deliver both. The APS-U provides high brightness and large coherence volumes at energies exceeding 40 keV, granting penetration into bulk specimens. At the HEXM beamline, a 16-meter sample-to-detector distance, state-of-the-art x-ray optics (Hi-res mono and focusing lenses) are needed to resolve the fringes. resolves coherent fringes from micron-sized embedded grains — making high-energy BCDI (HE-BCDI) of bulk polycrystals experimentally feasible. Locating a grain of interest among hundreds of thousands in a millimeter-scale ceramic requires navigation. Far-field HEDM (ff-HEDM) indexes grain orientations, centroids, and grain-average strain across the full specimen volume, and identifies multiple accessible Bragg reflections from a target grain. Point-focus HEDM (pf-HEDM) resolves grain morphology and the orientations of immediately neighboring grains — establishing the boundary character context essential for interpreting intra-grain strain heterogeneity. Using ff-HEDM indexing, we demonstrate multipeak HE-BCDI on an embedded ~5 μm $SrTiO_3$ grain in a bulk ceramic, accessing independent strain tensor components and yielding intra-grain strain maps that directly connect nanoscale defect structure to the surrounding mesoscale microstructure.

Incoherent Diffractive Hard X-Ray Imaging (IDI) for Nano-Focus Characterisation and 3D Reconstruction

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Lensless X-ray imaging techniques allow for the characterisation of objects with nanostructures.

To access the three-dimensional (3D) structural information, the object typically has to be rotated in order to record multiple projections.

In the recent work of Radloff et al., X-ray fluorescence intensity correlations, excited by few-femtosecond pulses from a free-electron laser (FEL) at the Linac Coherent Light Source (LCLS), were employed to retrieve 3D structural information of a non-periodic sample, without rotation. At different positions along the beam focus, fluorescence emitted from a vanadium foil produced speckle patterns. The analysis of the second-order correlations revealed structural features of the sample, and 16 projections without rotation were obtained, allowing astigmatism to be resolved. The experiment demonstrated that real-space structural changes are encoded in FEL-induced fluorescence. This approach enables lensless 3D imaging of non-periodic samples through fluorescence intensity correlations, offering broad applications in materials science, chemistry, and nanotechnology.

The method can also be applied to additional datasets, for example, to study the beam focus.

Transferability of AI Analysis Between Different Experimental Systems

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There are now many machine-learning approaches for interpreting coherent X-ray speckle patterns. Following the work of Howarth et al. [1], we use an unsupervised deep-learning framework for automated classification of relaxation dynamics from experimental rheo-XPCS data without requiring prior physical knowledge of the system. In that work, the network was trained to classify dynamical regimes using two-time correlation functions obtained from colloidal suspensions under shear in a Couette viscometer.

In the present study we test whether such a model captures more general dynamical signatures by applying the trained classifier to a physically distinct system: surface-XPCS measurements of non-equilibrium dynamics during dewetting of polymer bilayer films on Si substrates. Rather than retraining the network, we apply the rheo-XPCS-trained model directly to the polymer dewetting data in a zero-shot transfer setting [2], asking whether features learned from shear-driven colloidal dynamics generalize to stress-driven thin-film evolution.

Both experiments produce two-time correlation functions that reflect heterogeneous relaxation processes, although the underlying microscopic mechanisms differ significantly. This comparison therefore provides a test of whether machine-learned representations derived from one XPCS experiment can generalize across experimental platforms. Beyond classification of the two-time correlation functions [2–5], we explore whether a rheology-trained model can provide insight into the evolving stresses that drive the dewetting process. More broadly, this approach examines whether a single trained network can serve as a general tool for identifying dynamical regimes across a wide range of non-equilibrium coherent X-ray scattering experiments.

ConvexAD: A geometrically regularized differentiable model for BCDI phase retrieval

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Bragg Coherent Diffraction Imaging (BCDI) [1] enables 3-D characterization of morphology and lattice displacements in single-crystal nanoparticles with high spatial resolution and strain sensitivity. However, high heterogeneous strain and low-signal conditions often prevent standard phase retrieval algorithms from converging, limiting the study of many functional materials [2].

In this talk, we present ConvexAD, a novel phase retrieval framework based on automatic differentiation (AD). By leveraging GPU-accelerated gradient calculations via TensorFlow, ConvexAD iteratively optimizes the object's shape and phase through gradient descent, minimizing the discrepancy between observed and calculated diffraction patterns. Unlike traditional alternating projection algorithms, this AD-based approach allows for flexible forwardmodel design and the seamless integration of regularization constraints.
The core innovation of ConvexAD is the parameterization of the object support using the half spaces method. This strategy explicitly enforces amplitude homogeneity and compactness by defining the particle as a convex polyhedron, drastically reducing the dimensionality of the optimization space and enhancing convergence in highly strained cases. Validations on simulated and experimental BCDI data demonstrate that ConvexAD achieves unprecedented robustness, successfully reconstructing particles where traditional iterative methods fail and opening new avenues for nanoscale strain imaging.

End-to-End Modeling of XMCD-FTH Experiment using Wavefront Propagation

O Chubar, J Dvorak, **An He**, *W Hu*

We report on the implementation of a comprehensive wave-optics simulation capability for Fourier Transform Holography (FTH) with X-ray Magnetic Circular Dichroism (XMCD) contrast, developed within the Synchrotron Radiation Workshop (SRW). This development enables users to perform end-to-end modeling of magnetic imaging experiments, starting from the undulator source through beamline optics to the final holographic reconstruction. To support realistic XMCD-FTH simulations, we extended the SRW framework to handle helicity-dependent optical constants and implemented an efficient resampling strategy to resolve nanoscale mask features with minimal computational overhead. We present representative simulation results based on the CSX beamline at NSLS-II, demonstrating the framework's ability to predict interference contrast and reconstruction resolution as a function of beamline parameters. This tool is designed to assist beamline scientists and users in experimental planning and mask design, providing a rigorous way to evaluate imaging performance under realistic coherence conditions.

Characterization of a Ti64 tie clip made by metal injection moulding using coherent X-ray imaging

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Computed tomography and ptychography have been carried out on a Ti6Al4V alloy made by metal injection moulding (MIM). This material possesses attractive mechanical properties compared with other titanium alloys and the work has been done to determine porosity, defects, and the morphology at nanometer resolution.

Tomography was carried out at the European Synchrotron Radiation Facility, BM05. The Ti6Al4V sample, extracted from a sintered tie-clip, was scanned at a pixel size of 2.5 μm at an energy centered around 97 keV by using a combination of aluminium and molybdenum filters. Porosity distribution of the investigated volume was calculated for discretized sections of the volume. According to these measurements, the porosity decreases as we move from the top of the specimen to the bottom. The inline phase contrast also shows that the elements are not uniformly distributed as shown by the dark and bright regions in figure.
A focused ion beam (FIB) was used to extract two samples of cylindrical shape with a diameter of 10 μm . Then Ptychography tomography measurements were carried out at the Diamond Light Source i13-1 beamline. The experimental setup made use of a monochromator to produce a beam of 9.7 keV. A probe size of 5 μm was obtained using a Fresnel zone plate lens. The sample was scanned on a grid of 220 by 40 points with a step size of 1 μm in the horizontal and 3 μm in the vertical. We will present the results obtained at nanometer resolution and the analysis.

Optimizing Multi-slice Ptychographic Tomography for High-Resolution X-ray Imaging

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Multi-slice ptychography overcomes the limitations of the single-slice approximation by explicitly modeling beam propagation through a specimen, effectively addressing multiple scattering. When combined with tomography, multi-slice ptychography theoretically offers the potential to relax angular sampling requirements by providing depth information at each projection angle. However, this sampling reduction benefit is seldom realized in experimental X-ray ptychography due to well-known inter-slice crosstalk artifacts.

Here, we systematically evaluate multi-slice ptychographic tomography (MSPT) using both numerical simulations and experimental X-ray datasets to establish quantitative guidelines for its application. We investigate how object thickness, the numerical aperture of Fresnel zone plate optics, and object initialization strategies influence reconstruction accuracy. Simulations reveal that an informed object initialization—such as a coarse tomogram derived from sparse-angle single-slice reconstructions—significantly mitigates inter-slice crosstalk and improves depth resolution. Crucially, this enhanced depth resolution enables accurate projection extension, where adjacent angular projections are calculated to increase angular density without requiring additional measurements. The findings also demonstrate that improved initialization enhances depth resolution even when the specimen thickness is below the depth-of-field limit. We further demonstrate the practical advantages of MSPT using experimental data from a 3D-printed test pattern. Compared to standard single-slice ptychographic tomography, the MSPT reconstructions show a substantial reduction in streak artifacts from angular under-sampling and higher structural fidelity.

Rapid X-ray Ptychography Using a Randomized Zone Plate

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High-resolution X-ray ptychography, in 2D and 3D, is increasingly used to connect nanoscale structures across mesoscopic distances [1]. Mapping 3D nanoscale structure of a mm-scale computer chip or brain sample would be major milestones, demanding huge data volumes acquired quickly. With the advent of diffraction-limited storage rings, it was recently estimated that 100 nm resolution ptychography could be scanned at a rate of 6,000 μm^2/s when using the fastest available detector at 110 kHz [1]. At this rate, a single 1 mm^2 ptychogram requires a few minutes, and a 1 mm^3 volume measurement would take weeks.

We show that replacing the focusing optic with a randomized zone plate (RZP) [2] could enable the 6,000 μm^2/s scanning rate target with a much slower framerate, alleviating a major experimental cost of rapid ptychography. The RZP greatly increases the beam size on the sample compared to a standard Fresnel zone plate with the same numerical aperture, allowing for much larger scanning pitch. We designed a RZP for the 12-ID-E beamline of the Advanced Photon Source (USA) which achieves a 130 μm^2/s scanning rate using a slow 33 Hz framerate. Using the high coherent flux available since the APS-U upgrade, the required exposure time is under 1 ms. With a 1 kHz detector, scan speeds of 4,000 μm^2/s become possible. Furthermore, upgrading the Dectris Pilatus detector at 12-ID-E to an Eiger would increase the field of view, allowing 20,000 μm^2/s scan speed. This would bring down the time to measure a 1 mm^2 image to under one minute, and large-volume 3D scans become possible.

A Multiplexed Reconstruction Framework for Grazing-Incidence Reflection Ptychography

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The ongoing drive toward higher-performance semiconductor devices has been accompanied by increasing complexity in both device design and fabrication. As a result, conventional inspection methods are becoming increasingly inadequate, creating a strong demand for nondestructive, high-resolution characterization of near-surface structures and interfaces. X-ray grazing-incidence geometry is particularly attractive for this purpose because of its high sensitivity to thin surface layers, such as EUV lithography structures. However, strong dynamical scattering effects pose a major challenge for developing ptychographic imaging methods that are both accurate and computationally efficient.
One way to reduce dynamical effects is to perform reflection ptychography at larger incidence angles. However, this greatly reduces the scattered signal. Here, we propose an extended ptychographic reconstruction framework applicable at low grazing angles, where multiple scattering becomes significant. We exploit the distinct responses of the probe and object to multiple scattering processes and incorporate them into the framework through a multiplexed formulation implemented using automatic differentiation. Using both simulations and experiments, we show that the proposed approach enables reconstruction even in the presence of considerable dynamical effects. Although the current framework does not fully account for all multiple scattering paths, it offers a practical route to low-angle reflection ptychography and may support faster data acquisition with stronger scattering signals and lower dose requirements. We further validate the method using both simulated and experimental datasets and benchmark it against a conventional approach.

Characterization of Beam Instabilities via Burst-Mode Ptychography

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Ptychography is a high-resolution lensless imaging technique, yet its performance is critically limited by beam instabilities, particularly those occurring within a single exposure frame. While these fluctuations typically degrade image quality, they encapsulate significant information regarding the beamline's mechanical environment. In this work, we demonstrate that burst-mode ptychography can serve as a high-precision diagnostic tool to quantify and localize such beam instabilities without requiring auxiliary hardware.

By utilizing temporally oversampled diffraction data from a Dectris Eiger 16M detector at the TPS 25A2 beamline, we successfully retrieved time-resolved displacement vectors. Our analysis reveals a dominant horizontal beam instability with a characteristic length scale of ~33 nm. Fourier analysis of the retrieved trajectories identified two distinct resonant peaks at 29 Hz and 38 Hz.

These findings were independently validated through direct detector power spectral density (PSD) analysis and knife-edge photodiode measurements. Furthermore, we identified the source of these instabilities as ground-borne vibrations amplified by the asymmetric upstream mirror support system. This study demonstrates that burst-mode ptychography not only achieves sub-10 nm resolution but also acts as a sensitive probe for diagnosing complex mechanical resonances, providing critical insights for stabilizing next-generation synchrotron light sources.

Coherent methods at NanoMAX, the hard X-ray nano-probe at MAX IV

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The NanoMAX beamline [1] was one of the first beamlines to be build and taken into operation at MAX IV, the first 4th generation synchrotron radiation source in the world. As nano-probe, the beamline relies on the coherent fraction of the X-ray beam to achieve the small X-ray focus and thus profits from the improved emittance of the source.
Nowadays the beamline features two endstations in user operation, with both endstation relying on KB-mirrors [2] [3] to achieve the nano-focussing. The more recently added imaging endstation (EH1) [4] with optics, samples and all detectors inside the same vacuum vessel is more restrictive on sample size and mounting, but offers the cleanest data for ptychography (2D and 3D) in forward geometry and X-ray fluorescence of lower energy emission lines. Cryo-cooling capabilities at this endstation are under development and are expected to be finished this summer.The more seasoned diffraction endstation (EH2) [5] houses the focussing optics in vacuum, but the sample and most detectors in air, which allows for various sample mounts and sample environments. A sample goniometer and freely positionable detector on a large robot arm allow for experiments in Bragg geometry as well as forward geometry. This flexibility allows the user to use the beam for forward- or Bragg- CDI [6] / holography [7] / ptychography [8] and XPCS [9] as well as mapping experiments (STXM, DPC, XRF, SAXS, WAXS) that use the small beam, but not the coherence of the beam. In this contribution we present details on the design of the endstations, their captabilities, key parameters to plan any experiment at the beamline and results obtained with the two endstations.

X-ray 3D imaging with ptycho-tomography of aerogel polymer foams for fusion energy

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The National Ignition Facility achieved a net gain in inertial fusion energy (IFE) which has prompted an over $10 billion investment in IFE companies. A challenge in fusion is optimizing target design that would allow for a more uniform implosion on the fuel. A proposed method to improve the efficiency of the fusion targets is to wick liquid tritium and deuterium fuel in aerogel (Dicyclopentadiene or DCPD) foam shell capsules which have low density but increase uniformity of the compression of the fuel to maintain the high gain and yield of the IFE target.1 However, it is critical to characterize the density of the aerogel foams with 3D high-resolution images to better inform IFE hydrodynamic models.

Ptycho-tomography is an x-ray imaging technique that combines the high-resolution capability of ptychography and 3D information provided by tomography.2,3 Ptychography is a coherent imaging technique which scans a coherent beam across a specimen.4 A stack of diffracted patterns from these illuminated spots are recorded on an x-ray detector which then reconstruct into 2D projections. The projections depict x-ray phase shifts through a specimen which are used for tomography to obtain 3D density mapping.

The aerogel foam was produced by General Atomics and is the specimen we have used for the ptycho-tomographic experiment. The experiment was performed using the Bionanoprobe beamline (2-ID-D) at the Advanced Photon Source in Argonne National Laboratory using 8.8 keV x-ray beam. Ptychographic imaging and x-ray fluorescence mapping was performed in vacuum and at liquid nitrogen temperatures. We obtained 558 projections with each at a different angle on the aerogel specimen using ptychography which are then used to generate a 3D tomographic image of the aerogel foam. Additionally, we also include fluorescent images to include element characteristics. With these 3D density maps of the foams, hydrodynamic modeling can be used to simulate the implosion of IFE.

Broadband high-resolution X-ray ptychography system spanning tender to hard X-ray regimes: Instrumentation and Applications

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We report the development of a broadband X-ray ptychography platform at the BL10U beamline of the 3 GeV synchrotron radiation facility NanoTerasu, enabling high-resolution imaging across the tender to hard X-ray regimes. The system employs advanced Kirkpatrick–Baez focusing optics in combination with a high-speed CITIUS detector, providing stable and efficient measurements over a wide energy range without the need for frequent realignment. To demonstrate its capability, we applied this platform to the investigation of light-element-based systems, including a CMOS image sensor and sulfur-containing polymer materials [3]. In the case of the CMOS device, ptychographic X-ray computed tomography (PXCT) performed at 4 keV enabled nondestructive three-dimensional visualization of the internal pixel structure. Key features such as silicon photodiodes and deep trench isolation structures were clearly resolved with a spatial resolution of 34.1 nm. The measurements further allowed discrimination between Si and SiO_2 regions, as well as identification of high-density regions attributed to high-k materials. In addition, spectroscopic PXCT measurements at the sulfur K-edge were conducted on sulfurized polybutyl methacrylate. By acquiring datasets at multiple photon energies, we reconstructed three-dimensional maps of electron density, sulfur distribution, and local chemical states, distinguishing contributions from S–S and S–C bonds. The analysis revealed significant nanoscale heterogeneity within individual particles and systematic structural differences depending on particle morphology These results highlight the potential of tender X-ray ptychography and PXCT as versatile tools for nondestructive nanoscale characterization. The broadband capability of the system opens new avenues for combined structural and chemical analysis of semiconductors, polymers, and energy-related materials.

Diffraction-Based Characterization of Strain and Structural Dynamics in the Defect-Engineered Topological Insulator Bi2Se3

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Since many quantum properties of interest in materials arise because of the underlying symmetry of the host lattice, structural characterization methods are crucial tools in understanding the properties of quantum materials. One such tool, x-ray diffraction, offers insight into structural information across many length and time scales. In this work we apply a suite of different diffraction-based techniques, both with and without algorithmic reconstructions, to understanding the structural properties of the topological insulator Bi2Se3 grown on high-miscut Al2O3. This structure inherently exhibits complicated quantum phenomena both in equilibrium and when pumped out of equilibrium. It has recently been shown that successful growth on high-miscut Al2O3 produces semi-periodic line defects in thin-films of Bi2Se3 that simultaneously stabilize a single twin phase across the film. Growing Bi2Se3 in this way is a method of modifying the underlying symmetry of the lattice by creating bands of strained material. The spacing of these defects allows for a unique exploration of the capabilities of different x-ray diffraction techniques that also provide valuable information of the underlying strain across multiple length scales. We show that by combining dark field x-ray microscopy and analysis of speckles arising from coherent x-ray diffraction the strain distribution across 100s of nm length scale can corroborate the results of Bragg ptychography (which gives closer to unit-cell length scale information) obtained using nano-focused x-ray beams. Demonstrating how mesoscale structures give rise to speckles can push the understanding of x-ray photon correlation spectroscopy and other coherent scattering-based techniques. Additionally, the dynamics of these structured films were probed using pump-probe dark field microscopy showing the characteristics of energy transfer into the substrate and in the thin film. Combining these data provides a complete view of Bi2Se3 and demonstrates what is necessary for data pipelines collecting diffraction-based information.

Detection of Two-Step Nucleation Pathway in Liquid Pd77.7Cu6Si16.3 Using Time-Resolved 4D STEM

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Direct observations of crystallization pathways for products with similar composition to the parent phase are challenging, as any observation technique needs both high spatial and temporal resolution and the ability to differentiate crystal embryos from the bulk liquid on the basis of structure alone. Coherent nanodiffraction in 4D STEM enables the structure of nanometer sized regions of real-space to be determined but has previously been limited by slow temporal resolution. New high-speed direct electron detectors have enabled 4D STEM scans of a real-space region with 256x256 scan positions in less than 2 seconds, allowing for observation of nucleation behavior.

We studied crystallization of Pd77.7Cu6Si16.3 metallic liquid, isothermally annealed in its supercooled liquid state in the STEM after heating from the glassy state. 4D STEM experiments revealed a two-step nucleation pathway where a stable, modestly ordered crystal embryo several nanometers in size first forms from the bulk supercooled liquid. Then, a fully crystalline phase with stronger order nucleates from within this embryo before growing to consume the bulk supercooled liquid. The two-step pathway was observed across a range of temperatures with nucleation rates increasing with increasing temperature. These results were obtained using unsupervised machine learning to process large, noisy 4D STEM datasets to locate the embryo and crystal structural signatures.

Sub-surface Temperature Evolution Mapping during Laser Powder Bed Fusion via In-situ XRD

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The thermal evolution beneath the surface of the melt pool during laser powder bed fusion (LPBF) significantly affects the solidification process, plays a vital role in microstructure development, and further influences mechanical properties of the additively manufactured (AM) parts. However, it is impossible to reveal the transient thermal evolution by the postmortem analysis. Even though multiple in-situ characterization methods have been developed previously to measure temperature, probing sub-surface temperature evolution is still a challenge. In this study, a method using nano temperature probe (stable nanoparticles embedded in metal matrix) is proposed to acquire important temperature information during melting-solidification process in LPBF process. The variation of lattice parameters of nanoparticles captured by in-situ XRD reveals temporal temperature change. With embedding nano temperature probes at different locations in the material and aiming the incoming x-ray correspondingly, spatial temperature mapping beneath the surface of the melt pool can be achieved. Our research provides a useful tool to investigate thermal effect of manufacturing conditions and has potential to be incorporated into automated manufacturing system for in-situ adjustment of processing parameters.

Design of a Dedicated X-ray Photon Correlation Spectroscopy Beamline for the Korea 4th Generation Synchrotron

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The Korea 4th Generation Synchrotron Radiation facility (K-4GSR), currently under construction, will provide highly coherent and ultrabright X-ray beams enabling advanced coherent scattering techniques. Among the planned instruments, the CoSAXS (tentative) beamline is designed as the first dedicated X-ray Photon Correlation Spectroscopy (XPCS) beamline in Korea.

The beamline is optimized to exploit the high transverse coherence of the K-4GSR source and to maximize speckle contrast for time-resolved studies of nanoscale dynamics in soft-matter, complex fluids, and energy materials. To enable flexible experimental configurations, the instrument will support sample-to-detector distances of up to 22 m for small-angle XPCS measurements. In addition, scattering angles up to 45 degrees will be accessible with sample to detector distances up to 10 m, enabling wide-angle XPCS capabilities.

Beam size and focusing conditions will be controlled using two transfocators equipped with high quality diamond compound refractive lenses (CRLs). This configuration enables flexible beam conditioning while minimizing wavefront perturbations and preserving the coherence of the X-ray beam. The overall design aims to provide a versatile platform for coherent SAXS and XPCS experiments at the upcoming K-4GSR facility.

X-ray photon correlation spectroscopy of vicinal oxide surfaces

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While the surface of a crystal is static at room temperature, the dynamic properties of surfaces are manifest at temperatures allowing adatom diffusion such that the remarkable, dynamic nature of defects at the surface, such as kinks and steps, becomes apparent. We performed in situ X-ray Photon Correlation Spectroscopy (XPCS) measurements near the anti-Bragg position (001/2) on heated SrTiO3 (001) substrates with different miscut angles [1,2]. The temperature dependence of the intermediate scattering function indicates that the surface migration velocity is higher, and the step-edge energy barrier is lower on the low-miscut substrate (0.05o) than on the higher-miscut substrate (0.3o). Atomic force microscopy measurements after buffered HF etching and subsequent in situ high-temperature annealing also confirm the gradual coarsening of terrace widths and the formation of a smooth, TiO2-terminated SrTiO3 (001) surface. Such coherent X-ray studies provide novel insight into the dynamics of perovskite surfaces – critical information in the field of complex oxide heterostructures.

Temperature-Dependent Nanoscale Dynamics in Epitaxial Hf0.5Zr0.5O2 Thin Films Probed by Coherent X-ray Scattering

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In contrast to the well-known perovskite-structured ferroelectric oxides, hafnia has a fluorite crystal structure, and ferroelectricity only appears in thin films as a metastable phase. Understanding the nanoscale processes that govern phase stability in hafnia-based ferroelectrics is essential for controlling their functional properties in ultrathin devices. Here we investigate temperature-dependent structural dynamics in epitaxial Hf0.5Zr0.5O2 thin films integrated in La(Sr)MnO3/HZO/ La(Sr)MnO3/Nb:SrTiO3 (001) heterostructures using coherent synchrotron X-ray scattering. Temperature-dependent diffraction measurements reveal systematic structural evolution with film thicknesses in the 2–7 nm range. Results of X-ray Photon Correlation Spectroscopy measurements conducted near the HZO Bragg reflections show pronounced temperature-dependent speckle behavior. At intermediate temperatures, the two-time correlation patterns exhibit intermittent, avalanche-like behavior indicative of metastable structural relaxations via discrete and collective events across multiple length scales, while higher temperatures show faster decorrelation times. These observations reflect coupled processes involving structural variants, ferroelectric domain configurations, and defect-mediated lattice fluctuations, highlighting the capability of hard coherent X-rays in probing the complex dynamics of metastable ferroelectric films.

Status and Plans for Hard X-Ray Coherent Scattering at LCLS-XPP

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The LCLS-II High Energy (HE) upgrade is ushering in a new era of ultrafast science by extending the facility's high repetition rate capabilities into the hard X-ray regime. Leading this transition, the X-ray Pump-Probe (XPP) instrument is slated to be the first hard X-ray instrument to complete its upgrade and commissioning for high repetition rate experiments. The core scientific activity at XPP remains centered on capturing transient structural changes in condensed matter and chemical systems via x-ray scattering and stroboscopic techniques. The high-heat-load optics and high-repetition-rate detectors also prepares the instrument to exploit X-ray coherence for advanced pump-probe and probe-probe applications.

Specifically, pump-probe coherent micro and nano diffraction will enable the exploration of localized ultrafast dynamics within heterogeneous materials. Furthermore, the integration of the compact split-delay optics allows for X-ray Photon Correlation Spectroscopy (XPCS) to probe both equilibrium and driven fluctuations at the atomic scale. Together, these enhancements position XPP as a uniquely capable platform for the coherence community in exploring complex matter.

MAX 4U- the first fourth-generation lightsource upgrade

Robert Aymeric

MAX IV Laboratory

In 2016, MAX IV inaugurated the world's first fourth-generation storage ring. With unprecedented performance, this new accelerator paved the way for a new era of X-ray science. Currently, four more fourth-generation light sources are in operation, with many more to come online by 2040. Overall, the accelerator community is making considerable advancements in Multi-Bend Achromat (MBA)-type lattices. This is to such an extent that, whereas MAX IV paved the way for fourth-generation light sources, we will have diOiculties competing with other synchrotrons in the future.

With this in mind, we developed our vision for the laboratory to strengthen our beamline capabilities and ensure the excellence, relevance, resilience, and leadership of Swedish academic and industrial research with X-rays for the next decades.

This is **MAX 4U**, and is our proposal to upgrade our 3 GeV storage ring [1]. MAX 4U will further reduce the 3 GeV ring horizontal emittance from the current 328 pm·rad to better than 75 pm·rad on the horizon of the early 2030s. Beyond an accelerator upgrade, MAX 4U oOers opportunities to improve beamline performance, keeping MAX IV a leading platform for accelerating science, discovery, and innovation.

[1] A. Robert *et al.***,** Eur. Phys. J. Plus **138**, 495 (2023)
[2] https://maxiv.lu.se/max4u

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