Light Source Enabled Science
Room 319 - Session LS-MoA

Light Source Enabled Science

Moderators: Alexander Gray, Temple University, **Juanita Hidalgo**, NYU

1:30pm **LS-MoA-1 Advancing the Sample Space to Elevate the Power of Resonant X-ray Scattering**, ***Philip Ryan***, Argonne National Laboratory, USA **INVITED**

Deploying *in-situ* strain withelectrical *multi-modal* x-ray scattering measurements has allowed for powerful experimental configurations deepening our understanding of complex quantum phenomena. Touching upon a few recent topics e.g., nematic behavior in Fe superconductors (1-4) and quantum paraelectric behavior in $SrTO_3$ membranes (5) I'll demonstrate the value-added power of investing in the sample space and overview our plans to explore dopant-vacancy color center qubit behavior with symmetry and strain combining photoluminescent spectroscopy and x-ray scattering.

The ability to measure and control structure, symmetry or domain population of a twinned system, like an orthorhombic crystal or magnetic orientated domains can be a critical sample control parameter to study intricate quantum behaviors. In the iron-based superconductor, electronic nematicity is coupled to both the lattice and the conducting electrons leading to both structural and transport measurements sensitive to nematic fluctuations. While spin driven nematicity is prevalent in Fe pnictides, the role of spin versus orbit in the chalcogenide nematic behavior has been under investigation. The consortium of electrical and x-ray scattering measurements keenly addresses the relationship of lattice, spin and orbital order in the nematic phase space. $SrTO_3$ is a ubiquitous prototype material but is itself an intriguing enigmatic host of quantum behaviors, using strain as a tuning parameter we investigate the transition from classical to quantum behaviors and consider the unbounded potential studies deploying this combination of strained single crystal membranes with resonant x-ray scattering.

1.Strain-Switchable Field-Induced Superconductivity, Joshua J. Sanchez [https://arxiv.org/search/cond-mat?searchtype=author&query=Sanchez%2C+J+J], et al., Science Advances 9, eadj5200(2023). DOI:10.1126/sciadv.adj5200 [https://doi.org/10.1126/sciadv.adj5200] 2.Suppression of superconductivity by anisotropic strain near a nematic quantum critical point, P. Malinowski, et al., Nature Physics, 1-5, (2020)3.Spontaneous orbital polarization in the nematic phase of FeSe. Connor A. Occhialini, et al., Nature Materials 22, 985 (2023). doi:10.1038/s41563-023-01585-2 4. The transport–structural correspondence across the nematic phase transition probed by elasto X-ray diffraction. J.J. Sanchez, Nat. Mater. (2021) 5.Li J., et al. The classical-to-quantum crossover in the strain-induced ferroelectric transition in SrTiO3 membranes. Nat Commun 16, 4445 (2025

2:00pm **LS-MoA-3 Monolithic 2D Multilayer Laue Lens Optics for Hard X-ray Nanoimaging**, ***Wei Xu***, *Zirui Gao, Weihe Xu, Nathalie Bouet, Juan Zhou, Hanfei Yan, Xiaojing Huang, Ming Lu, Mingyuan Ge, Yong Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) are promising X-ray optics for nanometer-scale, high-efficiency focusing in the hard X-ray regime. Achieving high-performance two-dimensional (2D) focusing requires precise angular and translational alignment of two sets of linear MLLs, involving eight degrees of freedom of motion. For nanoimaging with sub-10 nm resolution, the tolerance for the relative angular alignment between the lenses is approximately 0.01°. Such stringent requirements pose significant challenges for microscopy systems and have hindered the application of MLLs in synchrotron light sources. In this work, we present the development of an advanced generation of monolithic 2DMLLs that address these challenges through a microfabrication-enabled assembly approach.

The monolithic optics were assembled using a silicon-based micro-electro-mechanical systems (MEMS) template. The template incorporates microfabricated alignment and holding structures that enable precise control of the angular and lateral positions of the MLLs mounted on the template. By engineering the alignment microstructures, an angular alignment resolution on the order of a few millidegrees was achieved, which was characterized by white-light interferometry and validated by synchrotron X-ray measurements.

The performance of the monolithic 2D MLLs was demonstrated at the Hard X-ray Nanoprobe (HXN) beamline at NSLS-II using ptychographic imaging. High-resolution 2D imaging achieved sub-10 nm spatial resolution, as verified by Siemens star test patterns. Furthermore, the optics were used to perform nanoscale X-ray tomography, revealing internal interfacial grain boundary structures in a $CoFe_2O_4$-$Ce_{0.8}Gd_{0.2}O_2$-based mixed ionic-electronic conductors (MIECs) system with nanoscale resolution.

This work demonstrates an effective and robust approach to simplifying alignment while advancing the performance of 2D MLL optics. The new optics with high alignment accuracy represent an important step toward the development of monolithic 2D MLL optics for hard X-ray nanoimaging.

2:15pm **LS-MoA-4 Development of Advanced High-Speed Fly-Scan Technology for sub-10 nm Hard X-Ray Imaging at NSLS-II**, ***Weihe Xu***, *Takenori Shimamura,* Brookhaven National Laboratory*; Dmitri Gavrilov,* brookhaven National Laboratory*; Huijuan Xu,* Brookhaven National Laboratory*; Wei Xu, Hanfei Yan,* brookhaven National Laboratory*; Nathalie Bouet, Juan Zhou, Randy Smith, Jun Ma, Xiaojing Huang, Yong S. Chu, Evgeny Nazaretski,* Brookhaven National Laboratory

Multilayer Laue lenses (MLLs) offer significant advantages over traditional diffractive focusing optics, such as zone plates (ZPs), particularly in terms of efficiency when focusing hard X-rays to 10 nm and below. The resulting increase in photon flux density drives the need for faster fly-scan capabilities to minimize radiation damage and improve data acquisition rates.

To answer this challenge, we developed a next-generation scanning X-ray microscopy testbed designed for high-speed data acquisition. The system demonstrated sub 10-nm ptychographic imaging, and achieved data acquisition rates exceeding 1 kPPS (kilo-points-per-second) while being fully compatibility with the Experimental Physics and Industrial Control System (EPICS) environment used at NSLS-II.

This system, called RASMI (RApid Scanning Microscopy Instrument) [1], is a stand–alone microscope that uses a modular design to accommodate either two orthogonally arranged 1D multilayer Laue lenses (MLLs) or a single 2D optic—such as a zone plate or a monolithically assembled 2D MLL—for point focusing. RASMI supports both sample–scanning and 2D–optics–scanning modes of operation through the use of interchangeable modules. In the sample–scanning mode, the sample is moved during imaging experiments while the focusing optics remain stationary. This approach is insensitive to the structural variations in the incoming X–ray wavefront, ensuring consistent illumination across the entire sample. In the 2D–optics–scanning mode, the 2D optic is moved while the sample remains stationary. This approach can achieve higher scanning speeds, particularly when working with heavy or bulky samples, such as large environmental or in-situ/in-operando experimental cells. Both scanning modes use a laser interferometer as the fast-axis encoder for position data acquisition. The entire RASMI control system is EPICS compatible. The developed microscope can be operated in both time- or position-triggering modes with the maximum photon flux- and detector-limited rate of 1.25 kPPS. The 2D X-ray image results show ~6 nm resolution at sample scanning and ~8 nm resolutions at 2D optics scanning [2]. The developed fly–scan technology has already been implemented in the user instrument at the Hard X–ray Nanoprobe (HXN) beamline at NSLS–II. In this presentation, we also highlight preliminary work aimed at further increasing position–triggered data acquisition speeds.

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1. Weihe Xu, et al., *Rev. Sci. Instrum.* 95, 113705, Nov 2024
2. Weihe Xu, et al., *Optics Continuum*, 5, 3 937-943, Mar 2026

2:30pm **LS-MoA-5 A Beamline for Probing Morphology and Dynamics of Thin Film Materials at the Advanced Photon Source**, ***Joseph Strzalka***, Argonne National Laboratory

Feature beamline 9-ID at the recently upgraded Advanced Photon Source hosts the program in nanoscale structure, kinetics and dynamics, focusing on surfaces and interfaces of soft materials. The beamline is tunable over the range 6-25 keV, with highly coherent x-rays provided by a revolver undulator with a double crystal monochromator. Two transfocators focus the beam to about a 5 um spot size at the sample. A robust diffractometer allows for alignment of thin film samples in a variety of sample environments for operando studies in a horizontal grazing-incidence geometry. An in-air area detector captures wide-angle scattering (GIWAXS) while a large vacuum flight path with an in-vacuum pixel array detector accommodates sample-detector distances from 3- 20 m for GISAXS and also grazing-incidence x-ray photon correlation spectroscopy (GI-XPCS) probing

dynamics over time scales from 10^{-3} to 10^{3} s. Early experiments at 9-ID make use of these capabilities to study the structure and dynamics of organic mixed ionic electronic conducting materials, organic semiconductors, block copolymers for separation science and perovskite-based materials for energy applications.

Acknowledgments: This work would not be possible without contributions from the 9-ID CSSI beamline development team: Ray Ziegler, Jayson Anton, Sunil Chitra, Miaoqi Chu, Peco Myint,Jonathan Knopp, Luca Rebuffi, Xianbo Shi, Deming Shu, Sunil Bean, Ashish Tripathi, Chasen Wolford, Luis Diaz, Steven Kearney, Kevin Wakefield, Altaf Khan, Dana Capatina, Miaoqi Chu, Peco Myint, Hannah Parraga, Scientific Co-Leads Zhang Jiang and Jin Wang, and Dynamics and Structure group leader Suresh Narayanan and team member Hongrui He. We are grateful for collaborations with the groups of Prof. Jonathan Rivnay (Northwestern University) and Prof. Alamgir Karim (University of Houston), Prof. Po-Chun Hsu (University of Chicago) and Prof. Wanyi Nie and Prof. Hsinhan Tsai (SUNY Buffalo). This research was performed on APS beam time award(s) (DOI: https://doi.org/10.46936/APS-189194/60013707, https://doi.org/10.46936/APS-190153/60014220 , https://doi.org/10.46936/APS-190281/60014340 , https://doi.org/10.46936/APS-191475/60015201) from the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science user facility at Argonne National Laboratory, and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

2:45pm **LS-MoA-6 The Role of Artificial Intelligence and Spectral Databases in Minimizing Analysis Errors, Illustrated with EXAFS, XES, and Core Level Photoemission***, **Jeff Terry,*** Illinois Institute of Technology

We have developed artificial intelligence-based methodologies that can be used to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS), X-ray Emission Spectroscopy (XES), and core level X-ray Photoelectron Spectroscopy (XPS). These efforts address persistent reproducibility problems that slow research progress and inhibit effective technology transfer and manufacturing innovation in materials science and related disciplines.

Our initial work focused on the analysis of EXAFS spectra collected at synchrotron radiation facilities. A machine learning approach, based on a genetic algorithm, was developed to fit measured spectra and extract relevant structural parameters. In the current approach, a set of possible chemical compounds, represented by feff.inp input files, that may be present in the sample. The algorithm then identifies the structural scattering paths from these candidate compounds that best reproduce the experimental measurement. The automated analysis searches for the primary EXAFS path contributors, calculates a goodness-of-fit value, and uses that metric to help identify the chemical moieties present in the material.

The resulting analysis package, EXAFS Neo, is an open-source Python code that uses Larch and FEFF to calculate and fit EXAFS paths. More recently, we have expanded this artificial intelligence framework beyond EXAFS to include XES and XPS analysis. These extensions make use of curated spectral databases for X-ray emission and core level photoemission, providing reference data that can be compared systematically with experimental spectra. By combining machine learning methods with database-driven spectral comparison, the analysis can reduce operator bias, improve consistency across users and laboratories, and provide more reproducible identification of chemical states, local bonding environments, and electronic structure signatures.

Together, these developments demonstrate how artificial intelligence, physics-based modeling, and experimentally grounded spectral databases can be integrated to minimize analysis errors in X-ray spectroscopies. The EXAFS Neo package and related information are available at: https://plutonium.phys.iit.edu/~jeff_terry/exafsneo.html or by contacting the speaker.

3:00pm **LS-MoA-7 Reliable Quantification of Oxygen Vacancies in Ferroelectric Hafnia Using Synchrotron-Based X-Ray Photoelectron Spectroscopy***, **Lucía Pérez Ramírez,*** *Tom Iung, Vineeta Yadav, Christophe Lubin,* CEA Saclay, France*; Uwe Schroeder, Florian Wunderwald,* Namlab, Germany*; Luis Azevedo Antunes, Alfred Kersch,* Munich University of Applied Sciences, Germany*; Tyson C. Back,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA*; Conan Weiland,* NIST*; Mickael Gros-Jean,* ST Microelectronics, France*; Nicholas Barrett,* CEA Saclay, France **INVITED**

Oxygen vacancy (V_O) is the most common anion defect observed in metal oxides. Its presence can effectively alter the electronic and physico-chemical properties of oxides thin films, thus determining the overall performances of entire devices built on these materials. This is the case of ultra-thin ferroelectric hafnium oxide (HfO_2) films used for emergent non-volatile memory and logic devices. As it has been demonstrated that V_O have a significant impact on the stabilization of the polar orthorhombic phase, responsible for hafnia's ferroelectric character [1,2], determining their global concentration in hafnia layers is crucial for optimal device engineering. Moreover, their migration during electrical field cycling can modify the internal field of the device, affecting the coercive voltage (E_C) and remnant polarization (P_R) values [3]. It is thus of major importance to have an insight on the V_O distribution profile along the hafnia ferroelectric film.

So far, X-ray photoelectron spectroscopy (XPS) combined with Ar^+ ion sputtering has been the preferred method for V_O quantification and depth-profiling, but this is an ill-chosen approach given its destructive character. Here, we show that the use of non-destructive, hard X-ray photoemission (HAXPES) using synchrotron radiation ought to be favored [4], in order to avoid the artifacts introduced by the sputtering process. The particular example of V_O quantification in hafnia appears as a good occasion to review the basics of core-level spectral analysis, focusing on the Hf 4*f* doublet, as widespread mistakes in literature with wrong fitting procedures unfortunately hinder the reliability of quantitative analysis. Finally, we disprove the erroneous assignation of one of the O 1s core-level peak components to the presence of V_O. We demonstrate that there is no concrete evidence to support the theory that associates this component to a charge transfer to second nearest neighbor oxygen anions upon a V_O creation. It is more judicious to assign the O 1s high-binding energy components to physisorbed or chemisorbed species. Our conclusions are supported by careful comparison between XPS/HAXPES experimental results and first-principles calculations [5]. We provide clear indications for reliable analysis and interpretation of the photoemission data, which should allow progress in materials engineering of ferroelectric devices.

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[2] Materano, M. *et al.* (2021) *Inorg Chem Front* 8(10), 2650-2672 [tel:2650-2672]

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3:30pm **LS-MoA-9 A Proposal for Fully Coherent nanoARPES: Probing Electronic Phase at the 10 nm Scale***, **Aaron Bostwick,*** *Chris Jozwiak, Eli Rotenberg,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Simon Moser,* Ruhr-University Bochum, Germany

Current nanofocused ARPES experiments have achieved ~100 nm spatial resolution, bringing the power of ARPES to microscopic samples and device geometries. Here we propose a new experiment— "Fully Coherent ARPES" — targeting spatial resolutions of 10 nm, where fundamentally new physics becomes accessible. At this length scale, true low-dimensional systems become directly accessible, including 1D edge states, quantum Hall states, and isolated nanotubes, as well as potentially 0D quantum dots and materials with nanoscale electronic phase segregation such as high-Tc_cc superconductors.

Achieving this resolution requires a move to higher photon energies (~200 eV) and a transmission rather than reflection geometry, with the increased coherent flux of the 4th generation synchrotrons offsetting reduced cross sections. When the beam spot approaches or falls below the electron coherence length, the photoemission process enters a fully coherent regime. In analogy with Fourier ptychography, interference effects can then be exploited to extract electronic phase variations induced by defects, strain, and structural inhomogeneities at sub-beam-size length scales — a capability with no current equivalent in electronic structure measurements.

4:00pm **LS-MoA-11 Probing Magnetic Interactions with Coherent Soft X-ray Scattering**, ***Andi Barbour,*** Brookhaven National Laboratory **INVITED**

The Coherent Soft X-ray (CSX) beamline at the National Synchrotron Light Source II (NSLS-II) welcomed its first facility users just over a decade ago, providing world–leading coherent X-ray flux in the soft X-ray regime. This capability has enabled fresh perspectives on a wide range of materials and has driven new insights, including the development and application of computational techniques that accelerate discovery—for example, deep-learning denoising models for X-ray Photon Correlation Spectroscopy (XPCS) data and Coherent Correlation Imaging (CCI). In this talk, I will highlight impactful results, along with the computational methods behind them, that reveal the spatiotemporal dynamics of magnetic systems, ranging from domain-wall motion to coherent rotational control of skyrmion lattices.

4:30pm **LS-MoA-13 Alloy Oxidation for Corrosion Mitigation: Synchrotron Based X-Ray-Photoemission Electron Microscope (XPEEM) Studies from NiCr to High Entropy Alloys**, *Keithen Orson,* University of Virginia*; Jurek Sadowski,* Brookhaven National Laboratory*; Yuran Niu, Alexei Zakharov,* Max IV Laboratory, Sweden*;* ***Petra Reinke,*** University of Virginia

Oxide layers are critical to protect alloys but design prioritizes bulk properties which leads to a narrow compositional and microstructural range to optimize environmental resilience. We study the initial reaction steps during the transformation of alloy to oxide in a kinetically limited regime (T < 800 ° C). We used XPEEM in the study of oxidation for binary (NiCr), ternary (NiCr with Mo or W), and septenary dual phase compositionally complex alloys (CCA).

XPEEM captures chemical, structural, and temporal evolution of the oxide for several grains or phases at the same time. The multi-mode capabilities access work functions, surface structure (m-LEED), and chemistry via XAS/ XPS and nanoscale resolution. The video rate time resolution allows operando studies with chemical sensitivity. The XPEEM studies are combined with (i) laboratory XPS, (ii) synchrotron based ambient pressure XPS, and, in the future, (iii) ToF-SIMS to access sub-surface alloy composition.

We will show oxidation as a function of crystallographic orientation for NiCr, and discuss the role of Mo/ W in moving the oxidation reactions to a preference for chromia over NiO. Several surface orientations were observed simultaneously and confirmed with EBSD analysis. The distribution of chromia islands was extracted from single-energy, time resolved images (operando mode) and hyperspectral XAS images. The analysis of the image stacks required alignments, distortion and brightness correction, linear combination analysis and cosine similarity to yield the composition Cr/Cr_2O_3 for each pixel as a function of oxidation time. The corresponding workflow and code are published. Significant differences are observed as a function of surface orientation but the endpoint for chromia island growth is controlled by Cr supply from the alloy (Figure 1). In contrast, for the ternary alloy (NiCr with Mo/W) the initial adsorption kinetics differ with orientation but chromia always grows in a layer-by-layer mode along [0001]. An atomic scale mechanism which favors specific O-adsorption sites contributes to this development.

For the two-phase septenary alloy $Al_{0.3}Cr_{0.5}Fe_2Mn_{0.25}Mo_{0.15}Ni_{1.5}Ti_{0.3}$ (Figure 2) we are interested in the speciation of elements in the two phases FCC and $L2_1$, their oxides, and the sharpness of the interface. We focus on hyperspectral XAS images for 6 out of the 7 elements for native oxide, clean and oxidized alloy. The alloy design achieved identical work function for both phases but the sharp interface at the boundary remains a breaking point. We will compare the element speciation between the phases in alloy and oxide and discuss the challenges of oxide identification with XAS.

4:45pm **LS-MoA-14 Bragg-Enhanced XAS for Monitoring Real-Time Reactions at Interfaces**, ***Karthika Madathil,*** Lawrence Berkeley National Laboratory (LBNL)*; Alisson Thill,* Universidade Federal do Rio Grande do Sul, Brazil*; Cheng Wang,* Lawrence Berkeley National Laboratory (LBNL)*; Baran Eren,* Weizmann Institute of Science, Israel*; Slavomir Nemsak,* Lawrence Berkeley National Laboratory (LBNL)

Heterogeneous catalysis is central to addressing global energy and environmental challenges. Detailed understanding of Interfacial phenomena during catalysis is limited via traditional X-ray absorption spectroscopy (XAS) due to low temporal resolution arising from the small volume of the interfacial region and the low signal to noise ratio. With Bragg-enhanced XAS (BEXAS) we incorporate diffraction optics into the material of interest using customized periodic nanopattern design enabling coherent addition of scattered intensity. Combining the element specific sensitivity of soft x-rays and intensity amplification from constructive scattering, we capture transient signals arising from chemical changes at thin interfaces. In this work we demonstrate BEXAS for monitoring real time interfacial dynamics in model cerium oxide samples. The evolution of XAS was monitored during heating and gas phase annealing of the sample. The experimental scattering data is compared with simulation results to connect the observed changes in scattered intensity to changes in interfacial chemical composition and structure during the reactions. BEXAS allows the expansion of XAS to the time domain, which is critical for understanding interfacial reactions and investigating transient states which are crucial for developing new catalysts.

5:00pm **LS-MoA-15 Novel Lattice-Matched Substrates for Scalable III-N Power Electronics**, ***Amitayush Jha Thakur,*** Argonne National Laboratory, India

Next-generation power conversion technologies will be central to a highly electrified energy system, motivating new materials and manufacturing approaches for power electronics built for speed, scale, and resilience. This work focuses on crystalline, electrically conductive substrates for III-nitride power electronics and the co-design of commensurate heterostructure interfaces for AlGaN growth. Lattice-matched substrates such as ScB_2 and $Ta_{1-x}Hf_xC$/TaC offer new opportunities for AlGaN heteroepitaxy by reducing interfacial strain while providing higher thermal and electrical conductivity than conventional substrates such as Al_2O_3 or SiC. ScB_2 is lattice matched to approximately $Al_{0.6}Ga_{0.4}N$, while $Ta_{1-x}Hf_xC$/TaC provides tunable lattice matching around $Al_{0.5}Ga_{0.5}N$. Preliminary X-ray characterization, including XRD, XPS, and XAS, probes crystallinity, orientation, chemical composition, charge state, and local electronic structure across multiple length scales, establishing an initial foundation for understanding structure–function relationships in novel AlGaN/substrate interfaces.

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