Session VII, September 10, Wednesday

L23

HARD X-RAYS WITH ORBITAL MOMENTUM, PROPERTIES AND DYNAMICAL DIFFRACTION

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Hard X-ray beams with non-zero angular momentum are generated by diffraction on a specially designed spiral-like zone plate. In the talk the simulations of the wavefield behind the zone plate will be presented based on a rigorous evaluation of the exact Huygens-Fresnel diffraction integral beyond the paraxial approximation. Unlike conventional vortex light in visible or IR range, vortex X-rays diffract in a crystal lattice showing peculiar diffraction effects demonstrated both theoretically and experimentally. Possible effect of an X-ray vortex beam on static poling of ferroelectric GeTe will be discussed.

L24

Study of local atomic structure of disordered materials with the aid of *in-situ* synchrotron experiments

ŠTÚDIUM LOKÁLNEJ ATOMÁRNEJ ŠTRUKTÚRY NEUSPORIADANÝCH MATERIÁLOV POMOCOU *IN-SITU* SYNCHROTRÓNOVÝCH EXPERIMENTOV

Jozef Bednarčík

Univerzita Pavla Jozefa Šafárika v Košiciach, Prírodovedecká fakulta

V tejto prednáške budú demonštrované možnosti vysokoenergetických fotónových zväzkov, produkovaných na zdroji synchrotrónového žiarenia 3. generácie PETRA III v DESY Hamburg, pri štúdiu štruktúrnych zmien vyvolaných tepelným spracovaním tesne pod teplotou kryštalizácie amorfnej zliatiny na báze Fe. Budú prezentované výsledky štruktúrnej relaxácie amorfnej zliatiny pri jej cyklickom tepelnom namáhaní. Získané výsledky budú analyzované pomocou dvoch prístupov: 1) v recipročnom priestore na základe pozorovania zmien tvaru prvého výrazného difúzneho maxima a následne 2) pomocou párovej distribučnej funkcie. Hlavný dôraz v príspevku bude kladený na uvedenie konceptu párovej distribučnej funkcie a jej využitia pri štúdiu silne neusporiadaných systémov.

L25

LIGHT-INDUCED PHASE SEGREGATION AND STRUCTURAL RELAXATION IN MIXED-HALIDE PEROVSKITES

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Mixed-halide perovskites are promising for high-efficiency multi-junction solar cells but are prone to light-induced halide segregation (Hoke effect), which alters their absorption spectrum and degrades optoelectronic performance. In this study we combined in operando and in situ X-ray scattering methods with complementary optical and electrical measurements to track structural changes, strain evolution, and domain morphology during illumination. Kinetic modelling using the Cahn–Hilliard formalism linked halide migration to observed diffraction peak broadening, indicating formation of Br-rich and Br-poor domains. Even after prolonged relaxation, residual strain and lattice parameter heterogeneity persist, underscoring the complex interplay between illumination, composition, and structural stability in these materials. Our results highlight the complex interplay between illumination, compositional changes, residual strain, and other factors such as humidity, single-crystal quality, or thin-film properties, emphasizing the need to fully understand all influences on the phase segregation effect and to mitigate them for the production of operationally stable devices.

CL1

ANTON PAAR, SAXSPOINT 500/700 - NEW EQIPMENT FRO SMALL-ANGLE SCATTERING

Jiří Špringer

Anton Paar

Anton Paar introduces SAXSpoint 500 and SAXSpoint 700, state-of-the-art laboratory beamlines offering unparalleled capabilities in SAXS/WAXS/GISAXS/USAXS/RheoSAXS analysis. Engineered for versatility, the SAXSpoint 500 is optimized for high-throughput and routine measurements, offering robust performance for quality control and standard research tasks. The SAXSpoint 700 extends capabilities with an ultra-low background design, enabling the characterization of weakly scattering and highly dilute samples at the highest scientific standards. SAXSpoint 700 features a spacious and innovative measurement chamber, allowing users to conduct experiments under ambient, non-ambient, and air conditions. The RheoSAXS integration in SAXSpoint 700 allows users to study structural and rheological properties simultaneously, combining the capabilities of SAXS with DSR 502 rheometer.

CL2

ENABLING NANOSCALE INSIGHT: ADVANCED X-RAY SCATTERING SOLUTIONS FROM XENOCS

Szymon Stolarek

Xenocs SAS, 1-3 Allée du Nanometre 38000 Grenoble France

Understanding structure at the nanoscale is critical to innovation across fields ranging from biotechnology to materials science. Founded with the mission to make advanced characterization tools accessible to researchers worldwide, Xenocs develops state-of-the-art laboratory solutions based on small- and wide-angle X-ray scattering (SAXS/WAXS) and X-ray imaging, enabling high-quality, multiscale structural analysis for both research and industrial applications.

This presentation will introduce two of Xenocs' flagship solutions: the Xeuss Pro and the Nano-inXider. Designed for maximum versatility, the Xeuss Pro is a modular SAXS/WAXS/GISAXS/USAXS/Imaging platform offering synchrotron-grade performance in the laboratory. It supports a range of X-ray sources—including microfocus sources with various target materials, MetalJet, and rotating anode (RAG) options—as well as a focused AuX

source for small-spot or high-resolution applications. With integrated USAXS and motorized SWAXS it enables fully automated and continuous measurements from atomic to micron scales. In addition, the InXight X-ray imaging module with dark-field and phase-contrast option further extends capabilities by revealing orientation, heterogeneity, and interfaces in complex materials. All these capabilities are seamlessly managed through the Xenocs Xplore control software, which provides an ergonomic interface for experiment planning, scriptable control (e.g. Python), and real-time equipment monitoring to track system performance remotely.

The Nano-inXider, by contrast, offers a compact, easy-to-use SAXS/WAXS system for routine nanostructural analysis. It combines a small footprint and intuitive operation with high-quality, reproducible data — making it ideally suited for quality control, process monitoring, and material development in both academic and industrial laboratories.

To complement these instruments, Xenocs provides XSACT Pro, an all-in-one SAXS/WAXS data analysis platform. It supports a wide range of analytical workflows including two advanced modules: one for AI-assisted shape classification and another for automated model fitting, helping researchers extract structural insights from complex scattering patterns quickly and reliably.

Figure 1. Xeuss Pro horizontal platform for SAXS/WAXS/GISAXS/USAXS and imaging alongside the Nano-inXider compact vertical system.

Trusted by leading academic institutions and companies across diverse sectors, Xenocs instruments accelerate material development and process optimization. Through high-performance, scalable, and user-focused solutions, Xenocs advances its mission: enabling nanoscale insight through continuous innovation.

Session VIII, September 10, Wednesday

L26

XRDLICIOUS: AN ONLINE TOOL FOR POWDER DIFFRACTION PATTERNS AND (P)RDF SIMULATIONS

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XRDlicious [1] is an online browser-based platform for computing powder X-ray diffraction (XRD) and neutron diffraction (ND) patterns, as well as partial and total radial distribution functions ((P)RDF), directly from crystal structure files. It supports common formats (CIF, POSCAR, XYZ, LMP) and can import data via file upload or integrated search in the Crystallography Open Database (COD), Materials Project (MP), and AFLOW. Multiple structures can be uploaded simultaneously, enabling direct comparison of computed diffractograms. Structures can be edited within the interface and exported in various formats. The tool also converts experimental diffraction data between wavelengths, d-space/q-space, fixed or automatic divergence slits, and supports conversion between XRDML (PANalytical) and RAS (Rigaku) formats into standard XY files and vice versa. Requiring no installation, XRDlicious runs on any device (computers, tablets, mobile phones) and across operating systems. Its intuitive interface and ease of use makes it promising for both research and teaching. The platform is freely available at xrdlicious.com, hosted on Streamlit community free cloud server, with source code and instructions for optional local installation at github.com/bracerino/xrdlicious.

1. (PREPRINT) Lebeda, M. et al. (2025). *Journal of Applied Crystallography 58*, https://doi.org/10.1107/S1600576725005370.

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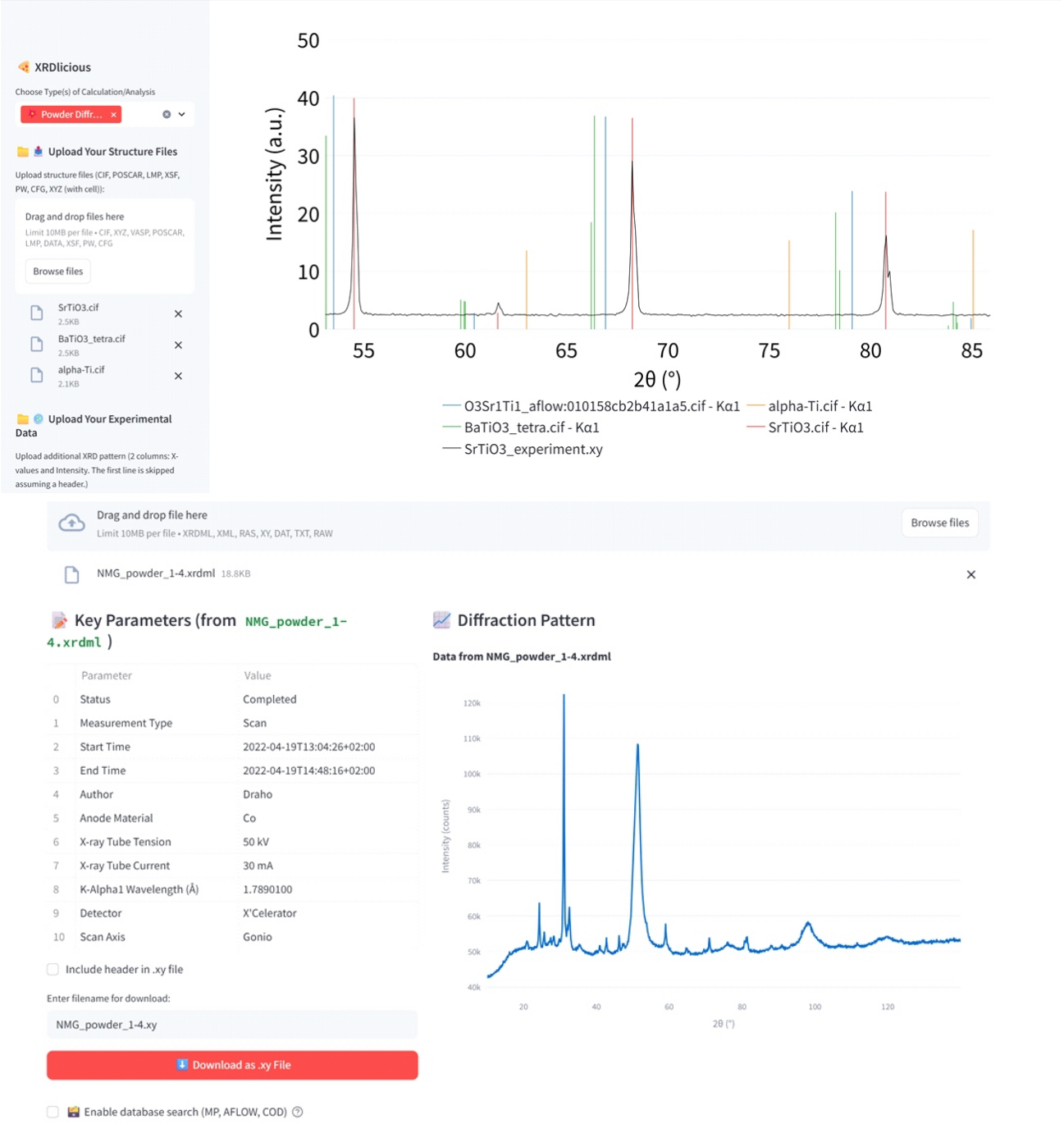

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3	End Time	2022-04-19T14:48:16+02:00
4	Author	Draho
5	Anode Material	Co
6	X-ray Tube Tension	50 kV
7	X-ray Tube Current	30 mA
8	K-Alpha1 Wavelength (Å)	1.7890100
9	Detector	X'Celerator
10	Scan Axis	Gonio

Figure 1. Example of XRDlicious output: calculated XRD patterns for multiple structures compared with experimental data, and demonstration of XRDML to XY file conversion.

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L27

BASIC CRYSTALLOGRAPHIC ALGORITHMS IN THE ML LANGUAGE

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Machine learning (ML) is increasingly finding applications in crystallography and materials science, enabling data-driven discovery of structural patterns, accelerating phase identification, and predicting material properties from complex diffraction and imaging datasets. In addition to these novel applications, traditional algorithms - used in crystallography for decades - are now being reimplemented using ML-based methods or simply executed within high-performance ML frameworks to benefit from their computing capabilities.

Among the next generation of scientists it is common a crystallography problem - that would be traditionally resolved by progressive analysis, followed by application of tailored numerical methods - is tackled by data-driven ML approach. While generic, unoptimized ML solutions often require more computational resources than traditional methods, the availability of optimized ML hardware and advanced software frameworks, built on robust mathematical libraries and developed by both the research community and industrial partners, can offer efficient alternatives.

This contribution aims to provide a gentle introduction to implementing several computational algorithms commonly used in the analysis of diffraction data in materials science and crystallography. The selected examples focus on well-understood, foundational algorithms that will be reformulated as neural networks. The process of solving these problems using data-driven approaches will be illustrated, including the full workflow and a discussion of its limitations, strengths, and potential ML-based extensions. Demonstrations will include peak parameter refinement using the least squares method, electron density map calculation, and a basic iterative algorithm for phase problem solving.

L28

MACE-INTERACTIVE: A BROWSER-BASED GUI FOR ATOMISTIC SIMULATIONS WITH MACE FOUNDATION MODELS

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Pre-trained foundation models in machine-learning interatomic potentials (MLIPs) allow researchers to perform accurate and efficient atomistic simulations without the need to search for or fit a potential for each studied system. These universal models approach the accuracy of density functional theory (DFT) while being orders of magnitude faster, making it feasible to study systems with even more than thousands of atoms, well beyond the practical size limits of DFT.

We have developed MACE-Interactive, a browser-based graphical interface designed to streamline calculations with the MACE MLIP foundation models [1]. The application supports multiple simultaneous structure uploads (POSCAR, CIF, LMP, XYZ with lattice), and presents calculated results in an easily readable way, allowing direct comparison between structures. Currently, the MACE-Interactive provides single-point energies, geometry optimizations, elastic properties, and phonon calculations, as well as genetic algorithm for identifying the energetically most favourable arrangements of substitutions or vacancies. The tool can also generate fully configured Python scripts based on the parameters set by the user in the interface for external console execution. The source code and installation instructions are provided at github.com/bracerino/mace-md-gui, with a video tutorial illustrating the application use and capabilities at: https://youtu.be/xh98fQqKXaI.

1. BATATIA, Ilyes, et al. A foundation model for atomistic materials chemistry. *arXiv preprint arXiv:2401.00096*, 2023.

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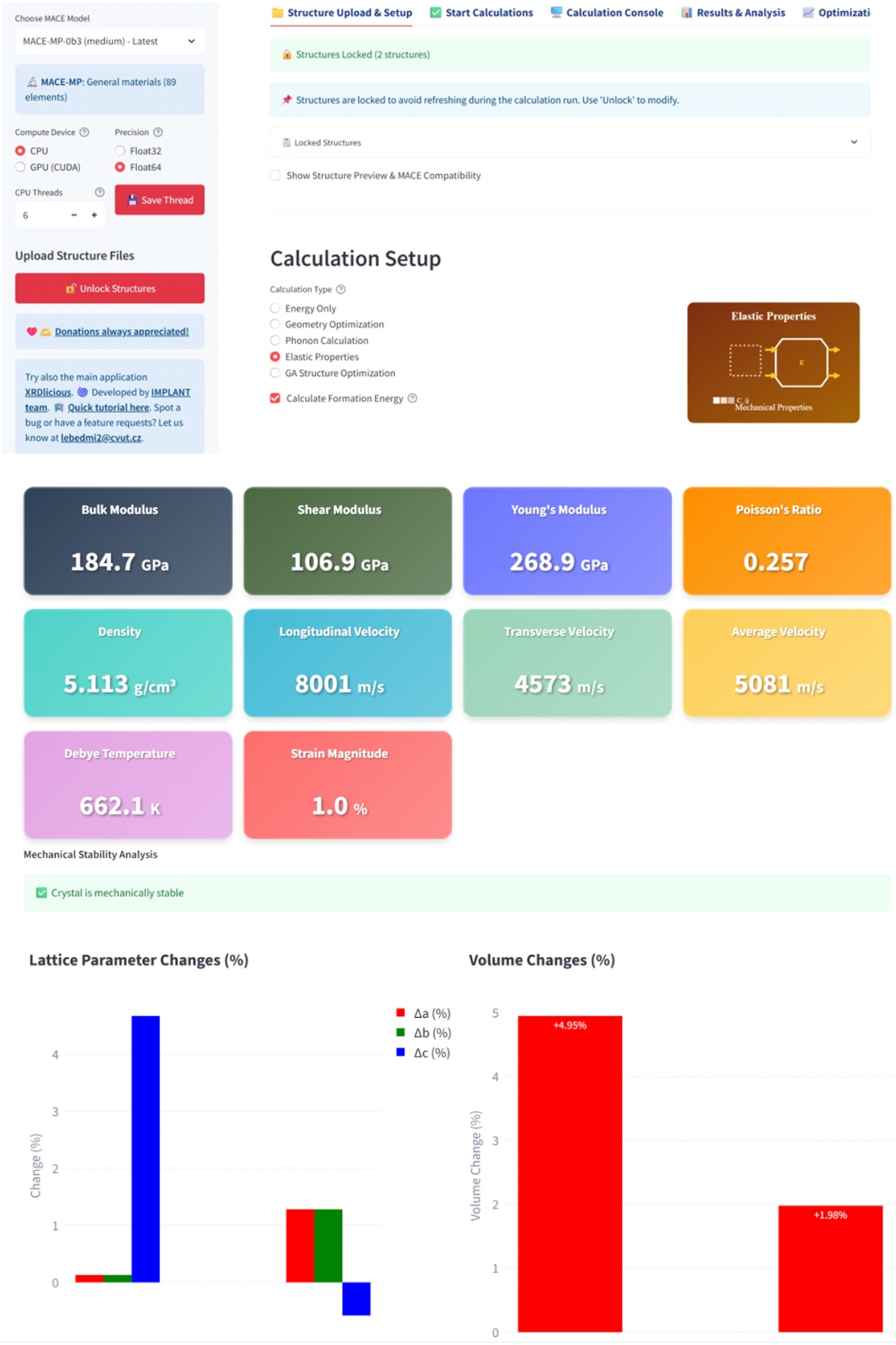

Figure 1. Example of MACE-Interactive: Calculation setup, computed elastic properties, and differences in lattice parameters before and after geometry optimization.