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EFFICIENT MODELING OF SINGLE CRYSTAL DIFFUSE SCATTERING

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Many modern materials exhibit a considerable portion of structural disorder, playing a key role in their functionalities. Routine crystallographic structure solutions based on positions and integrated intensities of Bragg peaks only reveal their average structure. In order to access the details of local atomic arrangements and their short-range correlations one has to study the shape of the Bragg lines and the diffuse scattering below and between them.

Unfortunately there does not exist any direct procedure permitting to extract such information from the observed diffuse intensities. The only way is to compare modelbased calculated intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices on nanometer scale by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on classical phenomenology (Landau formalism). Alternatively, one may approach the problem by reverse Monte-Carlo (RMC) modelling the displacement pattern in a supercell without making any assumptions on its origin.

With this progress in place the bottleneck has shifted from calculating supercell models with adequate displacement patterns to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue being the fact that scattering amplitudes from a lattice with displaced atoms cannot be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor $\exp(-i\boldsymbol{QR})$ being $\boldsymbol{Q}$-dependent. For this reason many efforts in recent years have been restricted to simple models on small supercells, which made the direct (naive) summation of the Fourier series viable [1,2], or to more involved models and RMC analysis of the pair distribution functions (PDF) [3-5], where the summation problém is reduced to a single dimension.

In this presentation we will introduce a novel approach [6] permitting to address this problem and to generate diffracted intensities from model supercells containing 10^6 atoms on seconds time scale. Even the computation of dynamic scattering functions $S(\boldsymbol{Q},\quad)$ necessitating to handle "movie" sequences of thousands of frames for the frequency transform can be addressed in an interactive manner.

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Session VI - Synchrotron radiation, Tuesday, June 21

L24

MICRO- AND NANO-SCALE 3D IMAGING AT SYNCHROTRONS

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Shortly after the first diffraction limited synchrotron source was built in Sweden, the ESRF upgrade took place and with this the second modern storage ring entered operation in Europe. The next one being the Swiss Light Source in 2025 we can ask the question what are the implications of the new technology for X-ray imaging. I will approach this question from various viewpoints including a discussion about the opportunities offered by the higher spatial coherence for nano and microtomography methods development. Through selected science cases I will attempt to indicate current trends in imaging methods development. Beside these trends in novel acquisition and reconstruction methods the weakest element in the workflow remains multidimensional image analysis, therefore I will conclude with commenting on this aspect of synchrotron imaging.

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MHZ MICROSCOPY AT EUROPEAN XFEL

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First MHz rate fourth generation hard X-ray XFEL source European XFEL [1] provide unique opportunity for characterisation of stochastic dynamics occurring in various systems either naturally or response is stimulated by an external force. High repetition rate of pulses (up to 4.5 MHz) together with high flux per pulse allow to record projected X-ray radiograms of dynamic samples and image more then million frames per second with high spatio-temporal resolution. Each such frame is illuminated using ultrashort exposure (fs scale) given by the X-ray pulse duration providing “frozen in time” snapshots of stochastic phenomena. This enable to film fast stochastic processes individual realisations in slow smooth motion. Experimental configuration of projection X-ray radiography is shown on Fig.1. Moreover, EuXFEL SASE1 undulator generate X-ray pulses with three orders higher number of photons per pulse (10^{12} photons) as compared to synchrotrons reaching hard X-ray range up to 24keV with ~20eV bandwidth. This unique performance allows for implementation of X-ray beam splitting schemes of multiprotection microscopy to obtain 3D snapshots per single pulse of dynamic objects sampled at MHz rate. We will present applications of recently developed MHz XFEL projection X-ray microscopy [2] applied for study of industrially relevant fluidic system behaving stochastically and we will present experimental results from recent characterisation of multi-projection MHz X-ray which is being developed under EIC-Pathfinder MHz-Tomoscopy project at SPB/SFX instrument [3].

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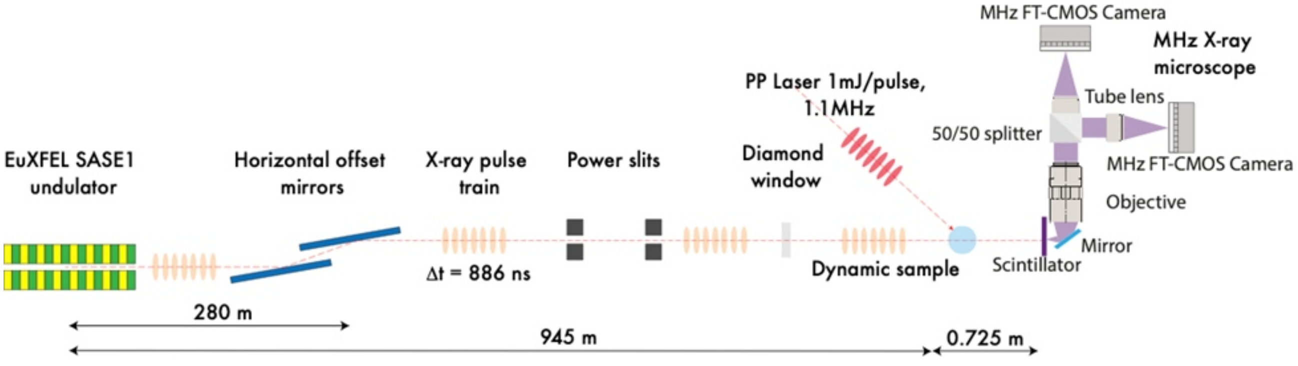

Figure 1. Experimental arrangement of MHz X-ray projection Microscopy at European XFEL SPB/SFX instrument.

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STRAIN MAPPING USING HIGH-ENERGY X-RAY DIFFRACTION

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Zr-based bulk metallic glasses (BMGs) exhibit extremely interesting mechanical properties such as superior strength (~2 GPa), high elastic strain limit (~2%), relatively low Young's modulus (50–100 GPa), high impact and fracture toughness, high corrosion resistance, excellent formability in the supercooled liquid region, wear resistance and biocompatibility [1]. Because of these unique properties Zr-based BMGs are emerging as a new class of metallic materials for biomedical, structural, and functional use.

Indentation techniques are used in many scientific fields ranging from biology to materials science and nowadays, they are at the heart of material nanoscience. In recent years the use of synchrotron radiation (SR) was increasing, and many diffraction techniques appears to be more desirable [2]. High-energy X-ray diffraction provides an effective method to observe the changes at the atomic level caused by mechanical treatment. Therefore, high-energy X-ray diffraction can be used to map the strain fields around an indent. Correlating the mechanical properties with the structure on the atomic and mesoscopic scale is a topic that promises a deeper understanding of the relevant processes during deformation. While the physics in crystalline materials is understood by large, the situation in case of amorphous solids is not advanced yet. Therefore, the connection of an indentation and diffraction gives a powerful tool for the delineation of composition-structure-property relationships and hence for material discovery and optimization.

In this contribution we present mapping of strain fields of indented Zr-based BMG using high-energy micro-diffraction technique. High-resolution spatially resolved scans in the vicinity of indents were done both ex-situ and in-situ.

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Information

Peter Oberta

ESRF

Petr Mikulík

ESUO

Session VII - Wednesday, June 22

Obituaries

Radomír Kužel
Vzpomínka na Václava Janovce
Obituary - Václav Janovec

Pavlína Řezáčová
Vzpomínka na Juraje Sedláčka
Obituary - Juraj Sedláček

Commercial presentations

Petr Marvan
(*Panalytical*)
Panalytical 2022

Boris Míč
(*MTM*)
Bruker 2022