Hard X-rays for coherent, time-resolved and imaging experiments at ALBA II

Report of Contributions

Contribution ID: **1** Type: **not specified**

Welcome

Monday, 4 October 2021 09:00 (10 minutes)

Primary author: ATTENKOFER, Klaus

Presenter: ATTENKOFER, Klaus

Contribution ID: **2** Type: **not specified**

Coherent synchrotron X-rays to enlighten the complexity of biological organs & organisms: a multi-scale and multi-modal approach

Monday, 4 October 2021 09:10 (30 minutes)

Over the past decades, synchrotron X-rays have open new avenues in biomedical research. The high degree of coherence and brilliance of synchrotron beams have made possible to reach unprecedented level of detail in the investigation of biological tissues through the application of advanced experimental techniques in in-vitro and in-vivo models. Ex-vivo studies allow optimizing experimental parameters and following the progress of diseases in sacrificed animals and/or excised tissues. Sophisticated hard X-ray setups have been developed to examine the morphology and alterations due to pathology and treatments at smaller and smaller scales, from micro- down to nano-scale, on both human and animal specimens establishing what is now indicated in the literature as 3D 'virtual anatomical histology'by X-ray imaging. However, ex-vivo investigations cannot access functional parameters that are fundamental in the understanding of a pathology. Elucidating the 3D structure and real-time function of organs in-vivo, at small length scales, is one of the most challenging applications of synchrotron radiation biomedical imaging. Dynamic measurements using methods such as X-ray phase-contrast imaging or multi-energy imaging are crucial to study organ structure and function (brain, lung, cartilage etc.). Thus, while exploring at higher and higher spatial resolution is key to understand some of the basic features and bio-mechanisms, 3D in-vivo imaging may allow gaining insight on the full organism and its physiological interconnections. These are the two opposite and complementary main directions along which synchrotron radiation can play a key role in biomedical imaging research filling the gaps of standard laboratory analysis techniques.
I am convinced and I will prove that in order to extricate and understand the complexity of biological systems (organisms) the application of multi-scale and multi-techniques approaches is fundamental and is the way to go. Results from selected scientific cases ranging from pathology detection and analysis, to the follow-up of the effects of novel treatments (including radio- and pharmacologic-therapies) will be presented. The key requirements of biomedical imaging as well as the main challenges in the field will be discussed.

Primary author: COAN, Paola

Presenter: COAN, Paola

Session Classification: Chair: Bart Bijnens

Contribution ID: **3** Type: **not specified**

Challenges for correlating STED and synchrotron XRF nano-imaging to explore metal functions in synapses

Monday, 4 October 2021 09:40 (30 minutes)

High spatial resolution correlative imaging approaches are needed to understand structure-function relationships in cell biology. These correlative approaches are particularly challenging for the study of biologically active metals in synapses due to (i) the labile binding of these elements, (ii) the nanoscale size of synaptic structures; (iii) the low concentrations of these elements. We correlated stimulated emission depletion (STED) microscopy of proteins and synchrotron X-ray fluorescence (XRF) imaging of metals, both performed at 40 nm spatial resolution, on primary rat hippocampal neurons. This correlative approach revealed the nanoscale co-localization of zinc and tubulin in dendrites, and the co-segregation of copper and F-actin in postsynaptic compartments. These results indicate new functions for zinc and copper in modulating the morphology of the neuronal cytoskeleton, a mechanism associated with synaptic structural plasticity. We will present and discuss the methodological workflow for correlative STED and synchrotron XRF imaging.

Primary author: ORTEGA, Richard

Presenter: ORTEGA, Richard

Session Classification: Chair: Bart Bijnens

Contribution ID: **4** Type: **not specified**

Hard X-ray nano-tomography for life sciences

Monday, 4 October 2021 10:10 (30 minutes)

Recent advances in hard X-ray microscopy make possible reaching new levels of resolving power in thick biological samples. Thanks to high brilliance coherent beams combined with cutting-edge nano-focusing optics and high precision tomographic scanning, X-ray holography can probe the 3D structure of up to millimeter sized tissues at tens of nanometers spatial resolution. This opens new horizons for life sciences research, enabling to bridge scales and address questions previously unreachable. A prominent example is deciphering the structure and logic of neuronal circuits and their evolution with aging and diseases. This talk will cover recent results obtained at the nano-imaging beamline ID16A of ESRF related to both fundamental life science questions and exploration of underpinnings and potential treatments for diseases such as Alzheimer's, diabetes, multiple sclerosis or cancer. The ID16A setup is equipped with a cryogenic system, enabling imaging of vitrified samples and offering better preservation from radiation exposure. Besides phase contrast imaging, the instrument includes high precision X-ray fluorescence imaging enabling to map and quantify the native elemental composition of cells and tissues. We will discuss the opportunities offered by these technologies, the current challenges to address, and perspectives in the context of the development of the fourth generation synchrotron sources.

Primary author: PACUREANU, Alexandra

Presenter: PACUREANU, Alexandra

Session Classification: Chair: Bart Bijnens

Contribution ID: **5** Type: **not specified**

Deep Learning for Synchrotron X-ray Imaging

Monday, 4 October 2021 10:55 (30 minutes)

X-ray imaging scans at today's synchrotron light sources can yield thousands of image frames per second at high resolution. Current and expected data volumes and rates necessitate having reliable, efficient, and fully automated data processing pipelines. Traditional image processes are difficult to be modeled and are not robust enough for the data with complex patterns and noises. Deep learning methods have proved the great potential for the image process. I will present our previous work of solving synchrotron X-ray imaging problems with deep neural networks, including three fundamental functions: image classification, image transformation, and a solver of inverse problems. I applied these functions for tomographic rotation axis calibration, low-dose tomography enhancement, super-resolution X-ray microscopy, X-ray image segmentation, missing angle tomography reconstruction, and phase retrieval. The relevant codes are released in the open-source software: Xlearn toolbox.

Primary author: YANG, Xiaogang

Presenter: YANG, Xiaogang

Session Classification: Chair: Bart Bijnens

Contribution ID: **6** Type: **not specified**

X-ray three-dimensional magnetic imaging, the future is brilliant!

Monday, 4 October 2021 11:25 (30 minutes)

Over the last years, we have worked towards developing methods to fabricate and characterize three-dimensional magnetic structures. Specifically, we have combined X-ray magnetic imaging with new iterative reconstruction algorithms to achieve X-ray magnetic tomography and laminography [1-4]. In a first demonstration, we have determined the three-dimensional magnetic nanostructure within the bulk of a soft GdCo2 magnetic micropillar and we have identified the presence of Bloch points of different types [1, 3]. Subsequently, we have used the flexibility provided by the laminography geometry to perform time-resolved measurements of the magnetization dynamics in a two-phase micrometer size GdCo disk. Therefore, X-ray magnetic three-dimensional imaging, with its recent extension to the soft X-ray regime [5], has now reached sufficient maturity that will enable to unravel complex three-dimensional magnetic structures for a range of magnetic systems.

In this presentation, I will first give an overview of our recent results and review the current shortcomings of the magnetic tomography technique. Finally, I will discuss how diffraction-limited storage ring source, together with state of the art instrumentation, will allow three-dimensional magnetic nanotomography to thrive.

[1] C. Donnelly et al., Nature 547, 328 (2017), https://doi.org/10.1038/nature23006

[2] C. Donnelly et al., New J. Phys. 20, 083009 (2018), https://doi.org/10.1088/1367-2630/aad35a

[3] C. Donnelly et al., Nat. Phys. 17, 316 (2021), https://doi.org/10.1038/s41567-020-01057-3

[4] C. Donnelly et al., Nat. Nanotechnol. 15, 356 (2020), https://doi.org/10.1038/s41565-020-0649-x

[5] K. Witte et al., Nano Letters 20, 1305 (2020), https://doi.org/10.1021/acs.nanolett.9b04782

Primary author: SCAGNOLI, Valerio

Presenter: SCAGNOLI, Valerio

Session Classification: Chair: Bart Bijnens

Contribution ID: **7** Type: **not specified**

Round Table

Monday, 4 October 2021 11:55 (1 hour)

Session Classification: Chair: Bart Bijnens

Contribution ID: **8** Type: **not specified**

Use of Coherence Methods in X-ray Powder Diffraction

Monday, 4 October 2021 14:00 (30 minutes)

Multibend Achromat Upgrades are being developed at a number of Synchrotron Radiation facilities, including ALBA. By greatly reducing the beam emittance, the coherent fraction of the X-rays produced by the undulators is correspondingly increased. The "diffraction limit"is reached where all X-rays up to a certain energy cutoff are fully coherent. This energy is expected to move into the hard X-ray range, with the consequence that ordinary diffraction experiments, such as powder diffraction at the MSPD beamline, become coherent diffraction experiments. While imperfect optics and beam vibrations might obscure the coherent diffraction effects, there is strictly no formal way to lose the coherence. So it will be important for users of MSPD to know how their data may be affected by the coherence.
Of course, there are great opportunities to use Coherence Methods to extract more information from X-ray Powder Diffraction experiments. One common data analysis technique, called the Williamson-Hall method [1], plots the measured powder diffraction line widths against the total momentum transfer. The slope of this line is a widely used quantitative measure of "microstrain", attributed to local distortions of the crystal lattice within each powder grain. When the illuminating beam is made coherent, each Bragg peak recorded in a powder pattern acquires fine structure in the form of fringes surrounding the peak centre. These fringes can be analysed using the Bragg Coherent Diffractive Imaging (BCDI) method to obtain real space 3D images of the crystal grain complete with the local distortions appearing as the image phase [2]. In this way the microstrain can be imaged, grain by grain, in the powder diffraction sample.
Another commonly used analysis method is to calculate the Pair Distribution Function (PDF) and complete the analysis of the crystal structure in real space [3]. PDF is particularly powerful for nanocrystalline materials with grain sizes below 100nm. This often requires Reverse Monte Carlo simulation of the real space distribution of matter to "fit"the PDF. With coherent BCDI images of typical grains of the material, these simulations could be directly tested.
[1] G.K.Williamson and W.H.Hall, Acta Metall. 1, 22-31 (1953)
[2] Ian Robinson and Ross Harder, Nature Materials 8 291-298 (2009)
[3] Takeshi Egami and Simon J.L. Billinge , "Underneath the Bragg Peaks: Structural Analysis of Complex Materials"(Pergamon press, 2003)

Primary author: ROBINSON, Ian (UCL)

Presenter: ROBINSON, Ian (UCL)

Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **9** Type: **not specified**

Exploiting brilliance at cSAXS, the small-angle X-ray scattering beamline at the Swiss Light Source

Monday, 4 October 2021 14:30 (30 minutes)

Located at about 1 hour from Zurich, the Swiss Light Source is a 3rd generation synchrotron quite comparable in size with Alba. The coherent small-angle X-ray scattering (cSAXS) beamline exploits the brilliance of its undulator source to perform experiments such as scanning SAXS, in which the beam is focused to a spot of about 10 microns and the specimen is raster scanned. By collecting SAXS patterns at each scanning position, this approach produces 2D and 3D images of samples in which structural properties on the nanometer scale are probed at each of their pixels or voxels. By further selecting the coherent part of the beam, diffraction patterns can be inverted using phase retrieval algorithms in a technique called ptychography to produce images with a spatial resolution down to 10 nm. Although our measurements currently take many hours, a planned upgrade of the ring and the undulator is expected to increase the brilliance by about 2 orders of magnitude. This will offer opportunities to speed up the measurements or improve the resolution, but will also challenge us to develop more efficient data acquisition and analysis methods.

Primary author: DÍAZ, Ana

Presenter: DÍAZ, Ana

Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **10** Type: **not specified**

Time resolved computed tomography/tomoscopy

Monday, 4 October 2021 15:00 (30 minutes)

Time-resolved in-situ and operando tomography is increasingly moving into the focus of materials research. Improvements in time and spatial resolution will be presented, which allow for an analysis of fast phenomena and detailed 3D process imaging. We apply real-time in-situ tomography with acquisitions rates of up to 1000 tomograms per second, which we call "tomoscopy". The sample environment is composed of IR lamps or an IR laser for contactless heating of the X-ray transparent crucible made from boron nitride into which samples are placed. Temperature is measured and controlled using a pyrometer. We show how fast tomography can be combined with simultaneous energy-dispersive diffraction, which is of special interest in cases where structural or morphological changes are correlated with chemical reactions or phase transformations caused, for example, by temperature variations. Some recent results and case studies include: (i) An analysis of the growth and evolution of liquid metal foams, where knowledge about the mechanisms of bubble formation, growth and degradation is gained. (ii) The immiscible hypermonotectic reaction of AlBi10 (in wt%) alloy and (iii) dendrite evolution in AlGe10 (in wt%) casting alloy during fast solidification. (iv) The combustion process and the evolution of the constituents in a burning sparkler. (v) The structure and density of two metal foams over a long period of time and derive details of bubble formation and bubble ageing including quantitative analyses of bubble parameters with millisecond temporal resolution. The work is performed at our own facility at EDDI, Bessy II, Berlin as well as at the Tomcat beamline, SLS, Villigen.

Primary author: GARCÍA MORENO, Francisco

Presenter: GARCÍA MORENO, Francisco

Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **11** Type: **not specified**

Probing structure development during "in-operando" processes by time resolved simultaneous Small and Wide Angle X-ray Scattering with synchrotron radiation

Monday, 4 October 2021 15:45 (30 minutes)

Since the earliest application of synchrotron radiation to the investigation of soft condensed matter it became clear that time resolved Small Angle X-ray Scattering (SAXS) experiments enabled plenty of opportunities for precise "in-situ"structural characterization[1-3]. The simultaneous use of Wide Angle X-ray Scattering with SAXS (SAXS/WAXS) paved the way for an extensive plethora of experiments aimed to characterize "in-situ"and "in operando"a great variety of processes in which structural changes take place. Nowadays there are a great variety of processes for which the monitoring of the structural modifications occurring while operation can be of great interest in order to optimize the process. As an example battery performance or additive manufacturing (AM) are among the novel topics in which "in-situ"and "in-operando"studies can be significant[4, 5]. In spite of the effort done in this respect there is still room for further developments aiming to provide user friendly platforms mimicking as close as possible everyday life processing conditions. In this talk, different approaches and the corresponding methodology for performing simultaneous SAXS/WAXS with synchrotron radiation during "in-operando"3D printing of polymers will be presented. In particular Fused Filament Fabrication (FFF) is one AM method based on the continuous layer-by-layer deposition of a polymer molten jet produced by hot extrusion. Upon deposition, the polymer melt cools down and solidifies out of equilibrium. The crystallization conditions of the polymer jet have a direct impact on the mechanical performance of the fabricated piece. The results will be compared with other crystallization experiments in noble gases liquid jets[6]. It will be emphasized the importance for "in-situ"and "in-operando"time resolved experiments of an up- grade in NCD-SWEET beamline at ALBA aiming for larger area detectors for both SAXS and WAXS stations to improve the time resolution below 100 ms as well as developments for treatment of big data.

1 - J. Bordas, I. H. Munro, and A. M. Glazer, Nature 262, 541 (1976).

2 - H. E. Huxley, A. R. Faruqi, J. Bordas, M. H. J. Koch, and J. R. Milch, Nature 284, 140 (1980).

3 - G. Elsner, M. H. J. Koch, J. Bordas, and H. G. Zachmann, Makromolekulare Chemie- Macromolecular Chemistry and Physics 182, 1263 (1981).

4 - G. Santoro, J. Manuel Amarilla, P. Tartaj, and M. Beatriz Vazquez-Santos, Materials Today Energy 10, 23 (2018).

5 - A. Nogales, et al., Macromolecules 52, 9715 (2019).

6 - A. Schottelius, et al., Nature Materials 19, 512 (2020).

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Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **12** Type: **not specified**

Complex Systems and Coherent X-rays: A perfect match

Monday, 4 October 2021 16:15 (30 minutes)

X-ray Photon Correlation Spectroscopy (XPCS) is a spatio-temporal coherent X-ray scattering technique that probes slow collective dynamics at the nanometric and atomic scale based on the observation of fluctuating far-field speckle patterns [1].
This technique has been successfully applied to the investigation of the slow relaxation processes occurring in disordered materials undergoing dynamical arrest, aging and poliamorphic transitions such as glasses, concentrated colloidal suspensions and viscous liquids [2,3].
The advent of 4th generation synchrotrons will allow to extend dramatically the dynamical range of XPCS, opening the field to new ground breaking experiments. For the first time, it will be possible to explore microsecond fluctuations in hard materials undergoing heterogeneous dyamics, and to unveil the particle motion of complex materials under extreme conditions.
In this talk, I will present some examples on the relaxation dynamics in metastable complex systems and I will also illustrate some of the future scientific possibilities offered by 4th generation synchrtrons as ESRF-EBS and the future APS-U.

Primary author: RUTA, Beatrice

Presenter: RUTA, Beatrice

Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **13** Type: **not specified**

Quantitative and chemical nanoimaging of heterogeneous materials by 3D X-ray ptychography

Monday, 4 October 2021 16:45 (30 minutes)

The properties of functional composite materials are heavily a ected by the arrangement of the different material phases within their 3D structure. The ability of visualizing their structures with high sensitivity and nanometric spatial resolution can improve the engi- neering of these composites. Ptychography is coherent X-ray imaging technique that has revolutionized this type of characterization[1]. We will show that ptychographic X-ray computed tomography (PXCT) is the key imaging technique to reconstruct quantitative 3D images of heterogeneous materials in such a critical length scale and with rela- tively large field-of-view[2-6]. PXCT provides 3D images from which we can extract the localization of the different material phases, the intermaterial pore space[1,2], and the composition of each constituent material of the composite without the need of additional spectroscopic measurements[4,5]. We will present a few examples of applications such as the analysis of the structure of technical catalysts bodies for the oil industry[2,3], the quantitative characterization of the hydration products of cement pastes[4,5], and the characterization of metallic alloys for aerospace industry[6]. We will also be discussing rapidly the future possibilities of using coherent X-ray beams in the new generation of synchrotron sources and development prospects at ESRF's FAME and D2AM French CRG beamlines.

[1] J. da Silva et al., Opt. Express 23, 33812-33821 (2015). [2] J. da Silva et al., ChemCatChem 7, 413-416 (2015).
[3] J. Ihli et al., Nat. Communications 8, 809 (2017).
[4] J. da Silva et al., Langmuir 31, 3779-3783 (2015).
[5] A. Cuesta et al., J. Phys. Chem. C 121, 3044-3054 (2017). [6] J. Haubrich et al., Appl. Surf. Sci. 433, 546-555 (2018).

Primary author: DA SILVA, Julio César

Presenter: DA SILVA, Julio César

Session Classification: Chair: Mari Cruz García-Gutiérrez

Contribution ID: **14** Type: **not specified**

Round Table

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