

“Quantitative Imaging using X-Rays and Neutrons”



15 - 19 May 2017, Grenoble, France



Imaging techniques have seen an intense development using neutron and synchrotron radiation over the past 20 years, with brighter sources and more efficient detectors.

Beyond experimental aspects, the data analysis workflow is essential for an efficient and objective interpretation of experimental data. This school will discuss the creation and use of images, with the help of “best practice” and “bad practice” examples, from the definition of experimental parameters, the reconstruction algorithms, to data visualization.

Techniques: two and three-dimensional imaging, time-resolved experiments, absorption, phase-contrast, scanning microscopy, coherent diffraction imaging, ptychography...

The school will include one poster session, one day of practicals and one day of tutorials focusing on data analysis.

Image credits:

P. Ginter, V. Fernandez,
P. Tafforeau, E. Lehmann,
G. Viggiani, E. Andò

Invited Speakers:

Edward Andò
Georges-Pierre Bonneau
Stefan Brandstetter
Emmanuel Brun
Peter Cloetens
Marine Cotte
François Curnier
Barbara Fayard
Stefan Eisebitt
Manuel Guizar-Sicairos
Andrew King
Eberhard Lehmann
Federica Marone
Rajmund Mokso
Markus Osterhoff
Armando Solé
Paul Tafforeau
Alessandro Tengattini
Simon Zabler

Organizers:

Birgit Kanngießner
Cino Viggiani
Claudine Roméro
Claudio Ferrero
José Baruchel
Judith Peters
Vincent Favre-Nicolin



Hercules Specialized Course HSC19

Quantitative Imaging using X-rays and Neutrons

e pn science campus, Grenoble

15-19 May 2017

Organizing Committee

José Baruchel (ESRF)

Vincent Favre-Nicolin (ESRF)

Claudio Ferrero (ESRF)

Birgit Kanngießler (TU Berlin)

Judith Peters (Université Grenoble Alpes & ILL)

Claudine Roméro (ESRF)

Cino Viggiani (Université Grenoble Alpes)

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Programme

HSC19 Final Programme, 14-19 May 2017

	Sunday 14 May	Monday 15 May	Tuesday 16 May	Wednesday 17 May	Thursday 18 May	Friday 19 May			
	Room	ESRF Auditorium		Beamlines & MD-1-21		ESRF MD-1-21			
08:30		Introductory lectures on imaging techniques		Hands-on training		Specialized lectures	08:30		
08:45		Welcome					08:45		
09:00		Analytical Imaging <i>B. Kanngießer</i>	Quantitative Coherent Diffractive Imaging & Ptychography <i>M. Guizar-Sicairos</i>	Practicals id1, bm05, id6, id16a, id17, id21	Tutorials ESRF + ILL (in parallel)	3D metrology in geomaterials <i>A. Tengattini</i>	09:00		
09:15								09:15	
09:30			09:30						
09:45		Radiography & Tomography <i>F. Marone</i>	Coffee break				Bio-Medical Quantitative X-ray Imaging <i>E. Brun</i>	09:45	
10:00								10:00	
10:15								10:15	
10:30							Coffee break	10:30	
10:45								10:45	
11:00		Coffee break	Scanning Microscopies <i>M. Cotte</i>				PyMCA: quick overview & recent developments <i>V. A. Solé</i>	11:00	
11:15								11:15	
11:30		Hard X-ray Phase Imaging <i>P. Cloetens</i>				11:30			
11:45					11:45				
12:00			Lunch	Lunch	Lunch	Image correlation/4D analysis <i>E. Andò</i>	12:00		
12:15									12:15
12:30							12:30		
12:45						Lunch	12:45		
13:00		Lunch			Tutorials ESRF + ILL (in parallel)		13:00		
13:15							13:15		
13:30							13:30		
13:45						Industrial Imaging <i>S. Zabler (Fraunhofer)</i> <i>B. Fayard (Novitom)</i> <i>F. Curnier (Digisens)</i>	13:45		
14:00			Neutron Imaging <i>E. Lehmann</i>	Practicals id1, bm05, id6, id16a, id17, id21	Tutorials ESRF + ILL (in parallel)	Time resolved X-Ray Holography <i>S. Eisebitt</i>	14:00		
14:15								14:15	
14:30		X-ray Optics for Imaging <i>M. Osterhoff</i>	Coffee break					14:30	
14:45								14:45	
15:00								15:00	
15:15								15:15	
15:30		Coffee break						15:30	
15:45							Coffee break	15:45	
16:00			Visual Perception of Complex data <i>G.-P. Bonneau</i>				Tutorials ESRF + ILL (in parallel)	Fast & Ultrafast Imaging <i>R. Mokso</i>	16:00
16:15		Diffraction Contrast Tomography <i>A. King</i>							
16:30								16:30	
16:45						Round table	16:45		
17:00							17:00		
17:15							17:15		
17:30			Debate: can we trust our brain ? <i>B. Kanngießer + everybody</i>				17:30		
17:45		DECTRIS				Conclusion	17:45		
18:00	Welcome Barbecue	Poster session Wine & Cheese		X-ray Imaging & Paleontology <i>P. Tafforeau</i> ESRF MD-1-21			18:00		
18:15					Discussion, questions,...			18:15	
18:30								18:30	
18:45								18:45	
19:00								19:00	
19:15								19:15	
19:30								19:30	
19:45								19:45	
20:00							School Dinner		20:00

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Useful information

WIFI CONNECTION IN EPN CAMPUS SITE

WIFI network is available in all the EPN Campus areas (ESRF, EMBL, ILL, IBS and common buildings).

There are two ways to get the internet:

- Via 'EPN Visitors' network:
Login: your e-mail address (*as registered in the ESRF user account in User Portal*)
Password: your SMIS password in lower-cases (*password used to access the ESRF user account via the User Portal*)

or

- Via Eduroam network:
The ESRF, the ILL and the IBS are eduroam-compliant: users who have a valid account in another eduroam compliant institution can use this network.

MEETING ROOMS (see map)

The HSC19 lectures on Monday 15 and Tuesday 16 will take place in the ESRF auditorium located in the ground floor of the ESRF main building. On Wednesday 17 May at 6pm and Friday 19 May all day the lectures will be held in room MD-1-21.

PRACTICALS & TUTORIALS (see map)

Wednesday 17 May Practicals and Thursday 18 May Tutorials

You will find the composition of the groups in this booklet (📄Practicals & Tutorials).

It will also be posted in the ESRF entrance hall.

Participants in the HSC19 courses will be picked up:

- for Practicals at 08:45am and 01:45pm
- for Tutorials at 08:45am and 12:45pm & 03.30pm

from the ESRF entrance hall and accompanied to the appropriate places.

POSTER SESSION (see map)

The Poster Session will take place on Monday 15 May from 6pm to 8pm in the entrance hall of the ESRF with a Wine and Cheese buffet. The posters will be displayed on Monday 15 and Tuesday 16 May. Each poster will have a number ordered alphabetically. Material to fix posters to the panels will be provided by the organisers.

COFFEE BREAKS

Coffee breaks on Monday, Tuesday and Friday will be served in the entrance hall of the ESRF main building.

LUNCH - DINNER

All the lunches and the dinners from Monday 15 to Friday 19 May (except on Monday and Thursday evenings) will take place in the restaurant on site (see map).

Please wear the HSC19 badge to access the restaurant!

The School Dinner will be held at the restaurant 'L'Epicurien' in Grenoble (1 place aux Herbes, +33 (0)4 76 51 96 06). We will go to the restaurant by tram with a departure from site entrance at 7pm.

DINNER DOWNTOWN GRENOBLE



The Epicurien, 1 place aux Herbes, 38000 Grenoble (+33 (0)4 76 51 96 06)
Meeting at 07:30pm in front of the restaurant.

Please use the transport tickets provided by us.

Take the tramway line B 'Gières Plaine des Sports' from Grenoble Presqu'île terminus, on the avenue des Martyrs and stop at 'Ste-Claire Les Halles'.



On your way back, take the tramway line B 'Grenoble Presqu'île' until the last stop. Please note that the last tram is at 01:07am.



EPN SCIENCE CAMPUS – 71 AVENUE DES MARTYRS – 38000 GRENOBLE - FRANCE



Room MD-1-21

ILL

EMBL

ESRF

Restaurant

Guesthouse
Chalet

EPN campus
site entrance

Practicals & Tutorials
meeting point
Entrance hall

IBS

Towards
EPN Campus

From/to Grenoble

3

1

2

1

SHUTTLE FROM LYON AIRPORT
SHUTTLE FROM & TO GENEVA AIRPORT

2

SHUTTLE TO LYON AIRPORT

3

TRAM B – Stop « Presqu'île »
From Grenoble (direction « Presqu'île »)
To Grenoble (direction « Plaine des sports »)

3

Lecturers' abstracts

Lecturers

Birgit KANNGIEßER

Technical University of Berlin, Germany

Federica MARONE

Paul Scherrer Institute, Villigen, Switzerland

Peter CLOETENS

ESRF, Grenoble, France

Markus OSTERHOFF

University of Göttingen, Germany

Andrew KING

Synchrotron Soleil, Gif sur Yvette, France

Stefan BRANDSTETTER

Dectris Ltd, Baden, Switzerland

Manuel GUIZAR-SICAIROS

Paul Scherrer Institute, Villigen, Switzerland

Marine COTTE

ESRF, Grenoble, France

Eberhard LEHMANN

Paul Scherrer Institute, Villigen, Switzerland

Georges-Pierre BONNEAU

Université Grenoble Alpes, France

Paul TAFFOREAU

ESRF, Grenoble, France

Alessandro TENGATTINI

Université Grenoble Alpes, France

Emmanuel BRUN

INSERM, Grenoble, France

Armando SOLÉ

ESRF, Grenoble, France

Edward ANDÒ

Université Grenoble Alpes, France

Simon ZABLER

Fraunhofer Institute, Berlin, Germany

Barbara FAYARD

Novitom, Grenoble, France

François CURNIER

Digisens, Le Bourget du Lac, France

Stefan EISEBITT

Technical University of Berlin, Germany

Rajmund MOKSO

Max IV, Lund, Sweden

Analytical Imaging

B. Kanngießer

Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany,
Birgit.Kanngiesser@tu-berlin.de

Imaging of samples on different length scales has an increasing impact in the use of X-rays and in an increasing amount of disciplines. Besides the already for some time established Computer-Tomography and its newest variant X-ray fluorescence tomography, the growing use of imaging techniques is due to the experimental access of the phase in various methods. This opened the door further to a spatial description of material properties. The investigation of structure-function-relationships would not be imaginable without imaging techniques. This development is accompanied with new challenges in its methodological use and image interpretation by the various disciplines and its production of a new quality and quantity of data.

Common to all different imaging techniques is that the computer has become an essential component, if not the most important one, of the experiments. Evaluation of raw data and their visualization have to be seen as integral component of the experiments. Quantity and quality of measurements are nowadays essentially determined by computer operation. The aspect of quantity, so the production of enormous amounts of data, is actually a widely discussed challenge at large scale facilities requiring new concepts of data storage and data representation on site. The “Big Data” subject appears in a specific form. The other aspect, the one of quality, is fundamentally determined by computer programs. For example, defining spatial resolution has to distinguish between instrumentally achieved, spatial resolution and the one produced by reconstruction techniques. Shortly, the standardization and validation of the various imaging techniques is necessary. *Otherwise the door to pure imagination will be opened widely.*

The fact that images in science are highly artificial and at the same time, as visual experience, intuitively convincing renders scientific handling of images into a challenge. Especially the aspects of validation and standardization are important, and can only be achieved by a thorough understanding of the methods.

As in former times in science validation and standardization of emerging methods are important milestones, which we should go for analytical imaging.

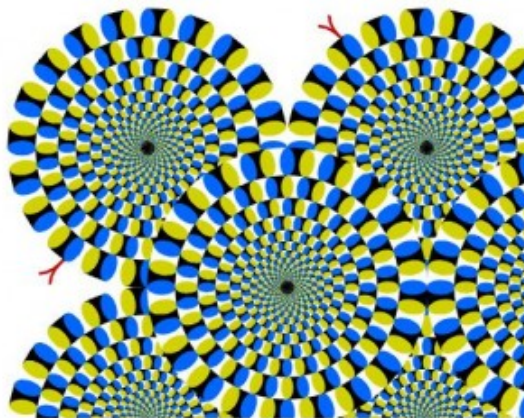


Image credits go to Akiyoshi KITAOKA.

Radiography & Tomography

F. Marone

Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland, federica.marone@psi.ch

Imaging with X-rays dates back to the late 1800 with the first radiography acquired by Wilhelm Röntgen. Nowadays, radiographic and tomographic imaging with X-rays is widely established. Modern radiology in the medical field and baggage screening at airport security checkpoints are just two examples which strongly rely on X-ray imaging. At third (and fourth) generation synchrotron sources, X-ray tomographic microscopy optimally exploits the brilliance and coherence of synchrotron radiation pushing spatial, temporal and density resolution paving the way to new scientific applications in different fields.

In this lecture, we will first outline the mathematical principles of tomographic reconstruction. Already in 1917, Johann Radon proposed the first mathematical formulation of tomographic image reconstruction, namely an exact solution for the reconstruction of a function from its line integrals. This formula is however only accurate for the ideal case, where the line integrals are exact, the projections are continuous and their number is infinite over π . In synchrotron based X-ray tomographic microscopy, these conditions are actually never satisfied. We will present traditional analytical reconstruction techniques [1] and alternative approaches based on iterative processes [e.g. 2, 3], discussing their advantages and disadvantages.

In a second step, we will also address some typical sources of error affecting the accuracy of the measurements and of the results during daily operation at tomographic microscopy beamlines, including edge-enhancement, local tomography and ring artefacts. We will finally present solution strategies for their mitigation and reduction.

We will conclude with a selection of recent examples from different fields, illustrating the capabilities and potential of X-ray tomographic microscopy.

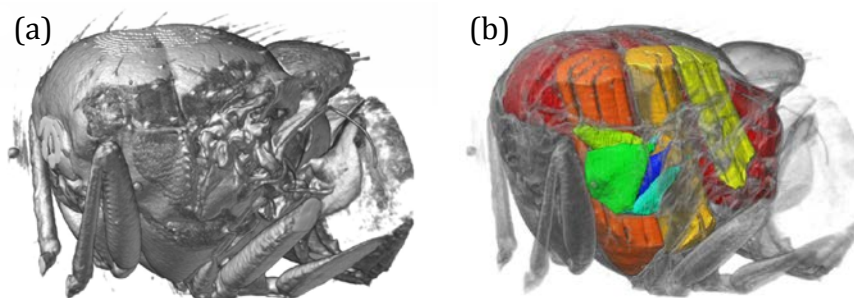


Figure 1: In-vivo imaging of a bowfly – External (a) and cutaway (b) visualization of the thorax: the steering muscles (green to blue) modulate the large output delivered by the power muscles (yellow to red) to enable highly complex wing motion patterns (after [4] which includes several 3D movies).

References

- [1] A.C. Kak & M. Slaney, *Principles of computerized tomographic imaging*. Society for Industrial and Applied Mathematics, 2001.
- [2] P. Gilbert, *Journal of Theoretical Biology*, **36**, 105-117, 1972.
- [3] J.A. Fessler, *IEEE Transactions on Medical Imaging* **13**, 290-300, 1994.
- [4] S. Walker et al., *Plos Biology* **12**, e1001823, 2014.

Hard X-ray Phase Imaging

P. Cloetens

European Synchrotron Radiation Facility (ESRF) - 71, avenue des Martyrs, Grenoble, cloetens@esrf.eu

In the hard X-ray regime, phase imaging is particularly valuable compared to attenuation based imaging due to its enhanced contrast and reduced dose requirements. Phase imaging is very suited to image soft materials, complex biomaterials and tissues, but it has also many applications in materials science. Thanks to the relatively weak interaction of X-rays with matter, quantitative imaging and tomography are possible. A number of X-ray phase contrast methods have been developed over the last decades [1-3], of which propagation based imaging remains very relevant due to the simplicity of the implementation and the high spatial resolution.

In propagation based imaging, phase contrast is generated by letting the beam propagate in free space after interaction with the object. The measured intensity is a Fresnel diffraction pattern, effectively recorded in the 'near-field' regime. A numerical procedure is required to retrieve the phase of the transmitted beam and, in combination with tomography techniques, to reconstruct the complex refractive index in three dimensions. Paganin introduced a popular single distance phase retrieval approach, valid for homogeneous objects and low spatial frequencies [4]. In general, the transfer of information from the object to the Fresnel diffraction pattern strongly depends on the spatial frequency. To completely retrieve the complex object transmission function, several measurements are therefore required corresponding to different effective propagation distances [5].

Propagation based phase imaging with a parallel synchrotron beam is a straightforward and an extensively used technique. The spatial resolution is limited in this case by the detector to about one micron. Low dose phase imaging at high X-ray energy is developed in particular for dynamic in-vivo studies. The low sensitivity for large lengthscales is counterbalanced by increased propagation distances, higher partial coherence and regularization in the phase retrieval process [6]. Magnified phase nano-tomography exploits the divergent beam behind a nanofocus to reach a spatial resolution of a few tens of nanometer [7]. It is a practical method to zoom non-destructively into the three-dimensional structure of matter and map the electron density quantitatively. X-ray phase imaging can further be used to improve the elemental quantification in 2D and 3D X-ray fluorescence imaging [8].

These powerful quantitative imaging capabilities will be illustrated by a number of applications and the combination of near-field Fresnel diffraction and ptychography will be addressed [9].

References

- [1] P. Cloetens, et *al.*, J. Phys. D: Appl. Phys. **29**, 133 (1996).
- [2] T. Weitkamp et *al.*, Opt. Express **13**, 6296 (2005).
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- [5] P. Cloetens et *al.*, Appl. Phys. Lett. **75**, 2912 (1999).
- [6] M. Langer, et *al.*, IEEE Trans. Image Process. **19**, 2428 (2010).
- [7] R. Mokso et *al.*, Appl. Phys. Lett. **90**, 144104 (2007).
- [8] E. Kosior et *al.*, J. Struct. Biol. **177**, 239 (2012).
- [9] M. Stockmar et *al.*, Scientific Reports **3**, 1927 (2013).

X-ray Optics for Imaging

M. Osterhoff

Georg-August University of Göttingen, Institut fuer Roentgenphysik, Friedrich-Hund-Platz 1, 37077
Göttingen, Germany, mosterh1@gwdg.de

With the advent of Extremely Brilliant Sources or diffraction limited storage rings, new challenges have to be mastered in optical design of beamlines, in sample environments including stable motorisation, and in X-ray detection. To fully exploit the brilliance increase of the upgraded ESRF promises two to three orders, photons have to be concentrated on the sample with higher accuracy and better stability than before.

X-rays interact only weakly with matter, and this applies also to optical elements. Opposed to the visible light regime, numerical apertures are vanishingly small and only reach values of 0.01 in very specific and challenging settings. Due to the short wavelength, many optics also suffer from challenges during fabrication.

We will learn the basics of X-ray optics and compare different geometries and principles of light focusing. Special emphasis lies on latest developments in nano-focusing optics that can concentrate hard X-ray beams down to few nano metres in two dimensions, and on the coherence properties of such optics. The applications in full-field imaging, scanning imaging, and as nanoprobe will be briefly discussed.

Mapping Polycrystalline Materials in 3D: Diffraction Contrast Tomography and Related Techniques

A. King

Synchrotron SOLEIL, L'Orme des Merisiers, 91192 Gif-sur-Yvette, France, king@synchrotron-soleil.fr

Many of the materials used in daily life, for engineering applications as well as many others, have a polycrystalline microstructure. This means that they are crystalline, and are made up of many crystallite grains. This grain structure can have an important influence on the properties and behaviour of the material. This level of structure, intermediate between the atomic scale and the bulk scale, has traditionally been difficult to characterise and study. One problem was the lack of techniques that can characterise such grain structures non-destructively and in three dimensions. The scanning electron microscope technique electron backscatter diffraction (EBSD) maps these grain structures but is limited to surface observations, so 3D characterisation is a destructive technique involving sectioning.

In recent years a new set of techniques responding to this requirement have emerged. These use the penetrating power of high energy X-rays, combined with diffraction, to reveal 3D grain structures in bulk samples. This means that grain mapping can be combined with in-situ experiments, allowing researchers to understand the interaction between processes and the material structure.

This talk will introduce one of these techniques, diffraction contrast tomography, developed at the ESRF [1]. The instrumentation, experimental method, and the standard data processing route will be presented, as well as more recent developments. The related family techniques, and their differences and similarities will be introduced more briefly. Some recent case studies will be shown to give an idea of the potential of the technique for materials science and other applications.

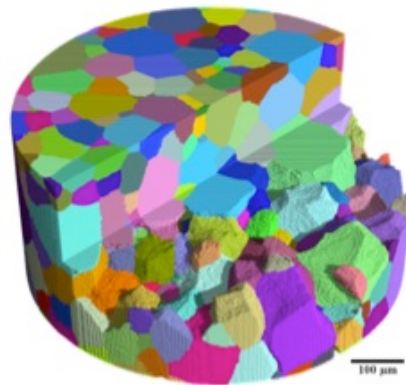


Figure 1: A 3D grain map from a titanium sample [2].

References

- [1] W. Ludwig, P. Reischig, A. King, M. Herbig, E.M. Lauridsen, G. Johnson, T.J. Marrow, J.-Y. Buffière, *Review of Scientific Instruments* **80** (2009) 033905.
- [2] M. Herbig, A. King, P. Reischig, H. Proudhon, E.M. Lauridsen, J. Marrow, J.-Y. Buffière, W. Ludwig, *Acta Materialia* **59** (2011) 590-601.

Detector Systems for Advances X-ray Studies

S. Brandstetter on behalf of the DECTRIS team

DECTRIS Ltd, Neuenhoferstr. 107, 5400 Baden-Dättwil, Switzerland, stefan.brandstetter@dectris.com

Hybrid Photon Counting (HPC) X-ray detectors [1,2] have transformed synchrotron research in the last decade by enabling noise-free detection and novel data acquisition modes. Two new HPC detector families promise to make even more ambitious science possible. First, PILATUS3 X CdTe detectors combine the advantages of HPC technology with the superior quantum efficiency of cadmium telluride (CdTe) at energies from about 10 keV to above 80 keV [3]. All other detector properties are identical to those of the successful PILATUS3 X series, e.g. a pixel size of $172 \mu\text{m} \times 172 \mu\text{m}$ and frame rates of up to 500 Hz. Second, EIGER detectors [4] offer smaller pixels of $75 \mu\text{m} \times 75 \mu\text{m}$, a frame rate of up to 9 kHz, and continuous read-out with 3 μs dead time between exposures.

In my presentation I will illustrate the advantages of the detectors results from three sets of experiments. First, we characterized detector properties like count rate capability, readout noise (restricted to cosmic background), and spatial resolution. Second, combining a nanofocus X-ray tube with a CdTe HPC detector we resolved features as small as 150 nm from test patterns (Fig. 1). This is a promising configuration for phase contrast imaging and nano computed tomography. Third, in experiments carried out with the EIGER X 500K at 9000 Hz at the CHX beamline at the National Synchrotron Light Source II in Brookhaven, United States, we demonstrated the combined power of a fourth-generation synchrotron light source and a state-of-the-art detector for coherent diffraction applications. Together, these results show how better detectors empower new fields of X-ray photon research.

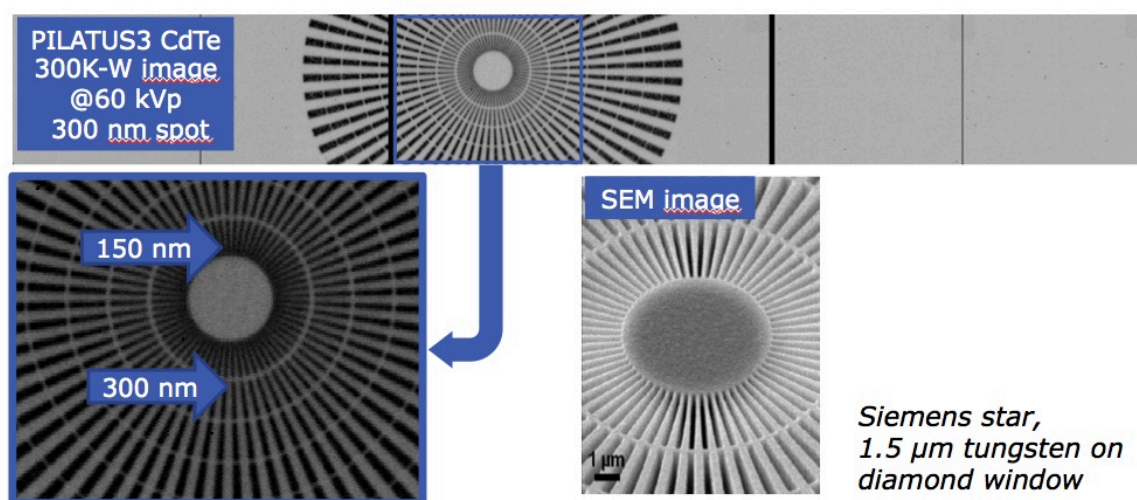


Figure 1: X-ray image of a test pattern using a PILATUS3 X CdTe 300K-W detector with 60 kVp

References

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- [2] T. Loeliger et al., IEEE Nucl. Sci. Symp. Conf. Rec., 610 (2012).
- [3] T. Donath et al., J. Phys. Conf. Ser. **425**, 062001 (2013).
- [4] R. Dinapoli et al., Nucl. Instrum. Meth. Phys. Res. **A 650**, 79 (2011).

Quantitative Coherent Diffractive Imaging and Ptychography

M. Guizar-Sicairos

Paul Scherrer Institut, 5232 Villigen PSI, Switzerland, manuel.guizar-sicairos@psi.ch

Coherent diffractive imaging (CDI) refers to a family of microscopy techniques for which imaging lenses are replaced by computations via iterative image reconstruction algorithms. The specimen of interest is illuminated by a beam with a substantial degree of transverse and longitudinal coherence, and intensity measurements are carried out in the far-field regime, effectively recording the intensity of the Fourier transform of the object exit wave. Ptychography is a scanning variant of CDI, in which the sample is scanned to overlapping illuminated regions and for each scanning position a far-field diffraction pattern is measured.

A main initial motivation to develop CDI and ptychography was to overcome limitations in resolution imposed by X-ray optics [1, 2]. However, other advantages have since then taken comparable importance, for example: precise quantitative estimates of local electron density, the possibility to reconstruct both phase and amplitude of the transmissivity which provides additional information about sample composition, and simultaneous characterization of the incident illumination wavefront. At the Swiss Light Source, we focus on the development and application of X-ray ptychographic nanotomography, see Figure 1.

I will provide an overview of the measurement strategies and reconstruction techniques for CDI and ptychography with emphasis on potential pitfalls or systematic errors that can arise during reconstruction or analysis of the data and how to adequately deal with them. For example, inherent degrees of freedom such as linear and global phase offsets, twin-image problem, scanning position inaccuracies, effects of partial coherence, misalignment of tomographic projections, and reliable estimations of resolution.

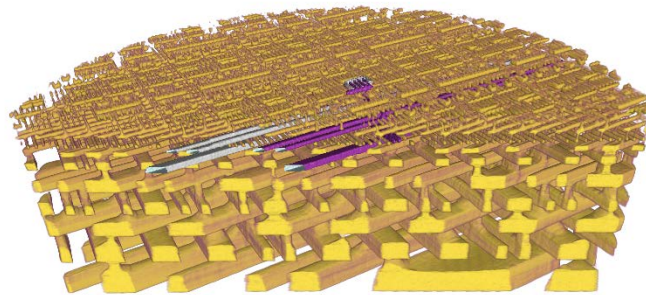


Figure 1: Rendering of metal layers from a segment of an integrated circuit measured with ptychographic nanotomography at cSAXS, Paul Scherrer Institut, Switzerland [3].

References

- [1] J. Miao, P. Charalambous, J. Kirz and D. Sayre, “Extending the methodology of X-ray crystallography to allow imaging of micrometre-sized non-crystalline specimens,” *Nature*, vol. 400, pp. 342-344, 1999.
- [2] H.M.L. Faulkner and J.M. Rodenburg, “Moveable aperture lensless transmission microscopy: a novel phase retrieval algorithm,” *Phys. Rev. Lett.*, vol. 93, no. 2, p. 023903, 2004.
- [3] M. Holler, M. Guizar-Sicairos, E.H.R. Tsai, R. Dinapoli, E. Müller, O. Bunk, J. Raabe and G. Aeppli, “High-resolution non-destructive three-dimensional imaging of integrated circuits,” *Nature*, vol. 543, p. 402–406, 2017.

Scanning Microscopies at the ESRF: a Synergy between Imaging and Chemistry

M. Cotte

ID21, ESRF, 71 avenue des Martyrs, 38000 Grenoble, France, cotte@esrf.fr

Many beamlines host scanning microscopes. All these beamlines have in common a basic principle: the beam is focussed and hyperspectral data are obtained by raster scanning the sample and measuring data over set of pixels -usually defined as 1D line, 2D map, 3D volumes. The acquisition resolution is directly determined by the probe size. A major characteristic of the different scanning microscopes is the type of technique(s) implemented for data collection. At the ESRF, scanning microscopes offer various contrasts: X-ray fluorescence will provide information about elemental composition; X-ray absorption spectroscopy will provide information about the speciation of elements of interest (e.g. oxidation state, coordination); X-ray diffraction, in its different modes, will provide information about long range organisation of matter (e.g. identification of phases, crystal orientation, measurement of strain). Other less conventional techniques are also available such as X-ray beam induced current, X-ray excited optical luminescence, or infrared spectroscopy without mentioning off-line scanning techniques (electron microscopy and Raman microscopy). These different techniques can also be combined on the same sample, simultaneously or not, to get the complete knowledge of sample composition and organization.

The different scanning microscopes and beamlines can differ by many aspects such as beam size, energy range, sample environment, etc. making them more dedicated to certain types of samples and scientific cases. As an example, the ID21 platform offers at a single beamline μ XRF, μ XAS, μ XRD and μ FTIR which, for example, are regularly combined to reveal the complex chemical compositions of micrometric fragments sampled from artworks [1], [2].

This talk will present the different scanning microscopes at the ESRF. Beamline capabilities will be illustrated with recent examples.

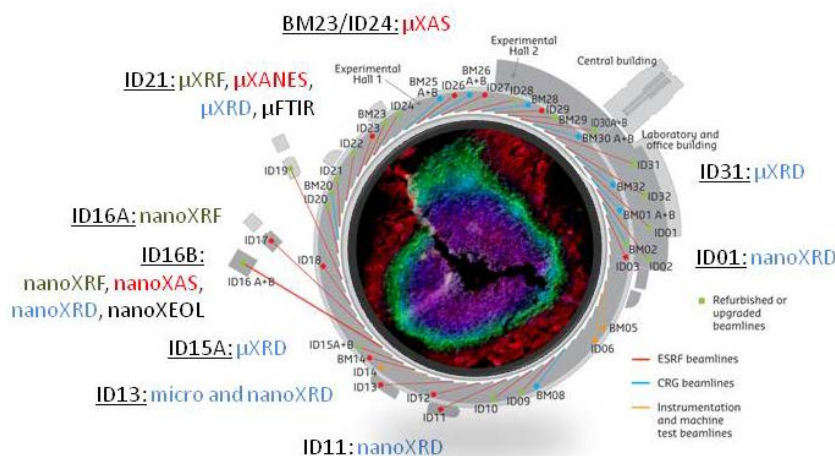


Figure 1: The different scanning microscopes at the ESRF

References

- [1] M. Cotte, J. Susini, V. A. Solé, Y. Taniguchi, J. Chillida, E. Checroun and P. Walter, *Journal of Analytical Atomic Spectrometry*, **23**, 820-828 (2008).
- [2] M. Cotte, et al. *Journal of Analytical Atomic Spectrometry*, **32**, 477-493 (2017).

Neutron Imaging

E.H. Lehmann

Neutron Imaging & Activation Group (NIAG), Paul Scherrer Institut, 5232 Villigen, Switzerland,
eberhard.lehmann@psi.ch

Compared to X-ray imaging techniques, neutrons can provide a lot of different and complementary options. Due to their higher penetrability for heavy materials and the large contrast for light isotopes (H, Li-6, B-10, ...) many applications in non-invasive studies are enabled. This has high relevance in industrial studies (fuel cells, batteries, moisture in porous media, metallurgy, ...) but also for many scientific fields (geo-sciences, plant biology, magnetism, nuclear technology,...).



Figure 1: Neutron tomography view of a carburetor (neither a CAD drawing nor a photo): metallic structures can very well be inspected with neutrons due to their high penetration and the high linearity in the attenuation coefficients

The talk will give an overview about the methodical progress in neutron imaging which has correspondence, but also uniqueness (e.g. driven by the magnetic moment of neutrons) in comparison to X-rays. The approach of data fusion between neutron and X-ray imaging is presented based on the installations at PSI.

Emphasis is given to the fact of quantification where the amount of involved materials should be derived with highest precision possible. Whereas for thin material layers an easy determination can be given according to the Lambert's-Beers law, for thicker structures some corrections for multiple neutron scattering and background removal have to be applied. Experimental techniques can help to overcome scattering artefacts too [1]. Comparison to other techniques (e.g. MRI) [2] are done to check and verify the quantitative accuracy.

References

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An Introduction to Visualization of Complex Data with a Visual Perception Point of View

G.-P. Bonneau

University of Grenoble and INRIA, CNRS UMR 5224, Laboratoire Jean Kuntzmann, Tour IRMA,
51 rue des Mathématiques, BP 53, 38041 Grenoble 9, France, Georges-Pierre.Bonneau@inria.fr

Despite many great advances in visualization research, we are still far from being able to intuitively convey the behaviour of complex scalar data through images. Part of the solution resides in developing theoretical and computing tools to extract and display meaningful features. It is equally crucial to take into account the strengths and the limitations of the human visual perception to derive efficient visualizations. This talk will first present a brief introduction to the domain of scientific visualization. The second part of the talk will be dedicated to the importance of visual perception in scientific visualization. We will present some basic facts about visual perception and explain how they can impact the way we look at visualizations. We will then dive more deeply into three research works in visualization in which perception is central. Two of these works [1,2] are dedicated to Direct Volumetric Rendering (DVR), and the perception of depth and transparency are crucial in these works. A third research work [3] concerns the visualization of uncertain scalar datasets using noise textures, and takes into account the contrast sensitivity of our visual perception system.

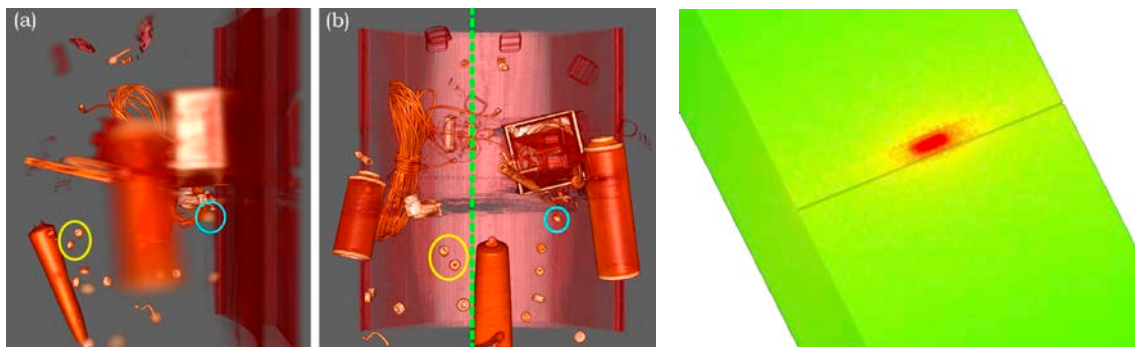


Figure 1: Depth blur is used to improve depth perception (left). Noise patterns convey uncertainty (right).

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Synchrotron X-ray Imaging and Palaeontology

P. Tafforeau

ESRF, 71 avenue des Martyrs, 38000 Grenoble, France, paul.tafforeau@esrf.fr

The first application of X-ray synchrotron microtomography on a fossil occurred at the end of 2000 at the ESRF. This research field originally appeared quite esoteric to many “classical” users of synchrotron. Nevertheless, it rapidly developed and became one of the very visible topics of synchrotron applications.

Many reasons can be invoked to explain this success, but the main one is clearly the application of phase contrast imaging to fossils. Originally, monochromaticity was the key aspect to scan fossils in order to get rid of beam hardening artefacts. Nevertheless, phase contrast rapidly appeared as the key to reveal internal structures of fossils with a sensitivity level not achievable with conventional machines, from sub-millimetric samples, up to specimens of dozens of cm.

Few years ago, monochromatic beams were abandoned on ID19 for palaeontology and were replaced by high quality tuneable polychromatic beams. These configurations can cover energy range from 19 keV up to 250 keV, are perfectly stable, have nearly no defects in the wave front and then high coherence level. Their bandwidths are narrow enough to make beam hardening not detectable in most of the cases. The high flux, coupled with specific detectors development, dramatically increased scanning speed and quality, as well as the maximum size of samples.

Unexpectedly, the development of high quality polychromatic phase-contrast imaging was also the key to reduce drastically the X-ray dose on sensitive samples that may still contain traces of DNA. It is nowadays possible on ID19 to reach much better quality than conventional X-ray microtomographs with similar or even lower dose when necessary. High versatility and exceptional quality of synchrotron imaging explain the success of palaeontology at the ESRF, as well as on several other light sources worldwide. The EBS project should bring the ESRF to a tremendous new capabilities level and lead to a new synchrotron revolution for palaeontology.

Bayesian Inference and Algorithms for Large Scale Computed Tomography

A. Mohammad-Djafari

Laboratoire des signaux et systèmes (L2S), CNRS-CS-UPSa, 3 rue Juliot Curie, 91192 Gif-sur-Yvette, France, djafari@lss.supelec.fr

Computed Tomography is an inverse problem. Regularization methods have been used with great success in different applications. However, a few difficulties still remain: the choice of the regularization term; the determination of the regularization parameter; more accurate errors and measurement noise modelling and quantification of the remaining uncertainties in the computed solutions. Bayesian inference framework can bring the right and appropriate answers to these difficulties.

In this tutorial presentation, first a short review of classical analytical and algebraic iterative methods based on regularization is presented. Then, the basics of the Bayesian inference is reviewed and illustrated on a 2D X-ray Computed Tomography. The focus here would be on the different models of the errors and different prior models for the images to be reconstructed. As we will see, the main point is choosing appropriate prior models. In particular we will mention non stationary noise model and sparsity enforcing prior models, both in a common framework. In the last part, more specialized methods are presented for real implementation in large-scale 3D applications.

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X-ray Powder Diffraction Imaging

W. De Nolf

ESRF, 71 avenue de Martyrs, CS 40220, 38043 Grenoble Cedex 9, France, wout.de_nolf@esrf.fr

When discussing the field of X-ray imaging, one mostly thinks of imaging techniques which provide an image of the sample, often in 3D, representing the X-ray attenuation or electron density of the material (e.g. absorption CT, phase-contrast CT, coherent diffraction imaging, ptychography, holotomography). The contrast in these images will allow you to distinguish areas with different chemical composition to a certain extent but will not reveal the exact nature of the chemical components.

On the other hand, several traditional X-ray analyses aim at chemical speciation of bulk samples: elemental composition can be retrieved by X-ray fluorescence spectroscopy (XRF), crystalline structure by X-ray powder diffraction (XRPD) and chemical composition by X-ray absorption spectroscopy (XAS).

The purpose of the ID21 beamline is to turn these three methods into imaging techniques while preserving their speciation capabilities. In this tutorial, XRPD imaging will be discussed more in detail. Figure 1 shows two possible experimental setups that can be realized with a focussed X-ray beam ($1\mu\text{m}^2$ in the case of ID21) and a diffraction camera. Both aim at showing the distribution of crystalline material in a sample, either in projection or in a virtual cross-section. In this tutorial, special attention will be given to the identification of chemical compounds and how their distribution can be derived with XRDU [1] from the diffraction patterns produced in a scanning XRPD experiment.

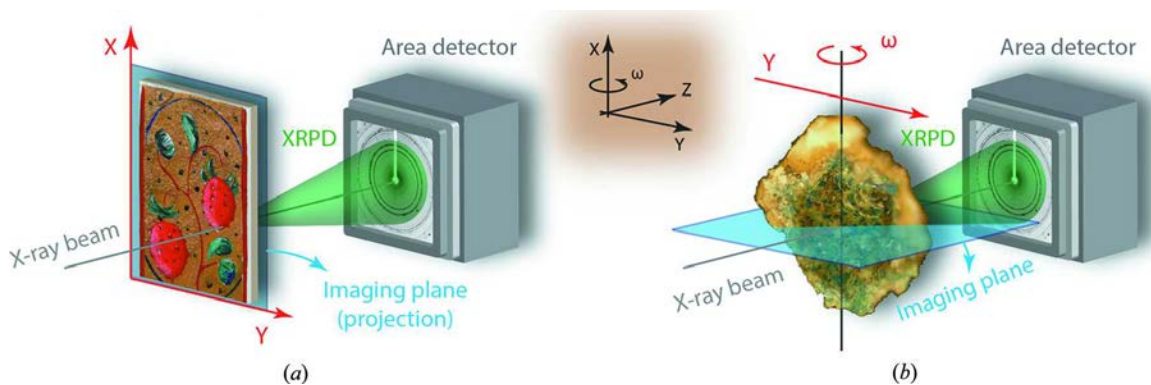


Figure 1: X-ray powder diffraction used for chemical imaging: (a) 2D scanning (b) tomography

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3D Metrology in Geomaterials

A. Tengattini, E. Andò

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000, Grenoble, France; ILL,
alessandro.tengattini@3sr-grenoble.fr

The understanding of the behaviour of geomaterials and porous media is at the very core of open scientific and engineering questions spanning from earthquakes to landslides and from bone implants to the safety of infrastructures. Despite the widespread interest that this broad class of materials has received since the dawn of science, they are still relatively poorly understood, partly due to their complex micro-structure.

Quantitative X-ray and neutron imaging techniques are at the centre of a veritable revolution in the field, also thanks to their capacity to provide non-destructive information of such evolving micro-structure. This specialised lecture will outline some key features of geomaterials and highlight the role that imaging has in their study, focusing on the key passage from qualitative observations to quantitative analyses.

Geomaterials can be broadly classified in continuum (e.g. rocks) and discrete (e.g. sands). In the former subclass, inclusions such as fractures or pores dominate their thermo-chemo-mechanical response. Key features determining the behaviour of granular materials include the position and morphology of the articles as well as their contact network. To extract this information, advanced image processing techniques such as segmentation are needed. This is a domain in rapid expansion also thanks to the overlapping interest with other fields such as medicine and automation.

Beside the characterization of a given state of the material, the non-destructive nature of X-ray and neutron imaging allows the study of their evolution during *in-situ* tests. These datasets are typically extremely rich in information although the development of robust quantitative analyses is often challenging and is at the edge of the ongoing effort in the community.

In several cases the confidence interval of the obtained measures is as relevant as the information itself, in particular when strings of tools are applied on images with varying degrees of noise. Its determination requires rigorous metrology studies on ground-truth cases.

Bio-Medical Quantitative X-ray Imaging

E. Brun

ESRF, 71 avenue des Martyrs, 38000 Grenoble, France, emmanuel.brun@esrf.fr

X-ray computed tomography (CT) is an invaluable three-dimensional non-destructive imaging method with numerous applications in life and material science. However, using conventional X-ray source CT confront limitations for soft tissue visualization. Phase-sensitive X-ray imaging can overcome some of these limitations and yield good contrast for soft-tissue structures.

In this presentation I will introduce the recent medical applications of Phase imaging that demonstrates the high potential of the technique.

Image Correlation/4D Analysis

E. Andò, A. Tengattini

Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, F-38000, Grenoble, France,
edward.ando@3sr-grenoble.fr

Quantitative X-ray and neutron imaging techniques are non-destructive, allowing the evolution of a scanned object to be followed by making repeated 3D measurements. This specialised lecture will cover some basic aspects of the analysis of 3D timeseries data (3D+t or 4D) with particular emphasis on the analysis of deforming media from materials science.

The 3D images resulting from X-ray and neutron tomography are 3D fields of the energy-lumped X-ray attenuation coefficient in the scanned area. If a sample is changing shape between two 3D images, this can be quantified as a displacement field, mapping one image into the other. This is most usually obtained with some variant of image or volume correlation which itself requires that the material has a visible, natural texture in the acquired 3D images.

The measurement of displacements less than one pixel is eminently possible with a number of different techniques, allowing the elucidation of very subtle material re-arrangements.

A number of challenging cases, which are being faced in the cutting edge of the field are the cases where between 3D volumes there are very large strains, fracture in a solid, breakage of objects and high-noise situations.

Recent work from the eminent group in Cachan has integrated image correlation with 3D image reconstruction which presents very interesting perspectives in time-saving during in-situ experiments, on the condition of parametrising the expected strain field sufficiently accurately.

X-ray Tomography in Industry: Current Status and Future Trends

S. Zabler

Fraunhofer IIS, Josef-Martin-Weg 63, 97074 Würzburg, Germany, simon.zabler@iis.fraunhofer.de

X-ray imaging is being used now for some decades to inspect and measure industrial products and parts on a large scale: cast alloy automotive components, steel welds and plastic parts. On the other hand the same technique is being used for luggage and food inspection. X-ray tomography, despite being available for about the same time, is still rarely used for the inspection of larger batches. Only now when computing power and the overall performance of scanners can perform inspection tasks within seconds, including measurement, volume reconstruction, registration and data analysis, CT is being considered for inline inspection in the production cycle. At the same time novel CT modes, such as phase-contrast or tensorial darkfield CT open up new fields of application in industrial CT.

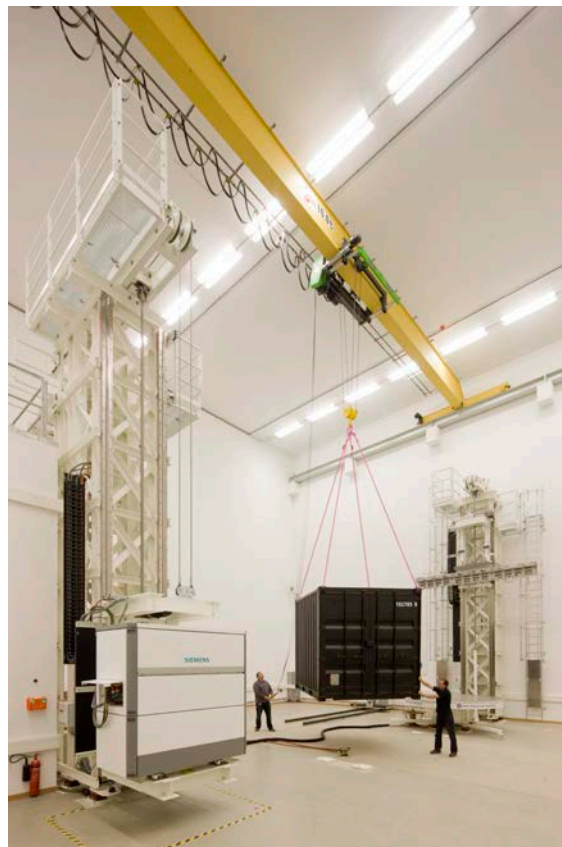


Figure 1: XXL-CT scanner at Fraunhofer EZRT Fürth

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Industrial Applications of Synchrotron Imaging Techniques

B. Fayard

NOVITOM, 1, place Firmin Gautier, 38000 Grenoble, France, barbara.fayard@novitom.com

Synchrotron sources offer a wide range of 2D/3D/4D imaging techniques that can find industrial applications in material characterization and non-destructive testing.

Synchrotron imaging techniques include X-ray micro- and nano-tomography, X-ray micro- and nano-diffraction, X-ray fluorescence microscopy or XANES microscopy. Most of these techniques allow dynamic characterization, where the visualization of 2D or 3D changes in the internal structure of the sample is made possible in real time while it is subjected to thermal, mechanical, chemical or biological stress.

Whether it deals with pharmaceutical and cosmetic products or composite materials for the aeronautic, the automotive or the energy industry, the benefits of such techniques are of great interest for industrial R&D that usually aims at a better understanding of the links between the process parameters and the final properties of the materials or the products.

The presentation will show few examples of applications and some experimental protocols and software tools which are still under development for a wider use of synchrotron imaging techniques in the industry.

Data to Measurement a Serpentine Road

F. Curnier

Digisens, 3D CT, 19 rue Lac Saint André, Bât. Le Fennec, 73370 Le Bourget du Lac, France,
francois.curnier@digisens.fr

Measuring and digitalizing objects is a wish of many imaging experts. However, linking computed tomography and metrology worlds is a tough task because of their very different areas of interest.

The subject of my short talk is about how to make this connection work.

X-ray Holography

S. Eisebitt

Max-Born-Institut and TU Berlin, Max-Born-Str. 2a, 12489 Berlin-Adlershof, Germany,
eisebitt@mbi-berlin.de

In this lecture, I will introduce basic concepts of static and time resolved X-ray holography. Furthermore, the combination of such techniques with spectroscopic information is discussed. Areas covered are: how is a holographic image formed in different geometries, how can this be experimentally realized using soft and hard X-rays, how can spectroscopic information be encoded, how can 3D information be encoded, how can temporal information be encoded? What general approaches are there to study the dynamics of processes down to ultrafast time scales with spatial resolution?

Fast & Ultrafast Imaging

R. Mokso

MAX IV Laboratory, Lund University, Fotongatan 2, 22592 Lund, Sweden, rajmund.mokso@maxiv.lu.se

In the last 15 years of tomographic microscopy at synchrotrons we experienced in average an order of magnitude improvement in the acquisition speed every three years. While in the early times the scan time of 60 minutes at 1-3 μm voxel size was the state-of-the-art, today we can achieve a temporal resolution of 20 ms.

Which are the main scientific drivers for this development? What technical and conceptual breakthroughs contributed to such a spectacular improvements? [1] Are we at the technical or physical limits of the spatio-temporal resolution? What will the future of diffraction limited light sources bring? These will be some of the questions I will reflect on in my lecture.

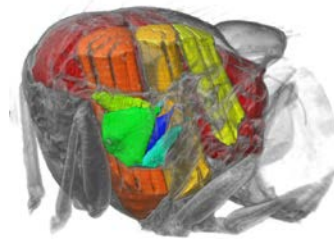


Figure 1: Tomographic reconstruction of the flight muscles of a blowfly during flight [2]. The 3D image represents a snapshot with a temporal resolution of 0.3 ms resulting in a 3D movie of the internal processing in the fly during flight.

References

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Practicals & Tutorials

Practicals

Wednesday 17 May 2017

Participants in the HSC19 courses will be picked up at 08:45am and 01:45pm for morning and afternoon sessions respectively from the ESRF entrance hall and accompanied to the appropriate place.

Beamline	Tutor	Title	Abstract
id01	M.I. Richard T. Schülli	Ptychographic wavefront reconstruction for coherent diffraction imaging studies	This tutorial will take place on the id01 beamline, specialized in imaging and strain studies using coherent X-ray diffraction methods and/or nano-diffraction. The practical will primarily focus on the quantitative characterization of the X-ray beam, using a standard target (Siemens star). If there is sufficient time, we will also perform Bragg coherent diffraction, which can be used to study strain in single nano-structures
bm05	V. Fernandez	propagation phase synchrotron contrast microtomography	Synchrotron microtomography allows the characterization of many kind of sample in various domain such as material science, biology or palaeontology, benefiting from the brilliance to greatly improve the signal-to-noise ratio. The coherence of the beam makes it possible to perform hard X-ray phase-contrast tomography and enhance the visualization of structures of similar density, by simply increasing the sample detector distance. During this practical, we will present the setup required to perform this technique and images a few object to demonstrate its interest.
id06	P. Cook	Dark-field Hard X-ray Microscopy at ID06	This tutorial will take place on the recently-constructed Hard X-ray Microscope (HXR)1. In dark-field mode, a Bragg reflected X-ray beam is used to image the crystalline phase, shape, orientation, and strain of grains in polycrystalline materials. The use of hard X-rays enables in-air analysis of thick samples, with the possibility to insert sample environments for in-situ experiments. The full-field approach provides recording times compatible with real-time measurements of events occurring in a few hours to days. This technique shows promise for the examination of complex hierarchical polycrystalline materials as found in metals, fuel cells, ferroelectrics, and in biominerals with exceptional spatial and angular resolution.
id16a	J.C. Da Silva	Quantitative high-energy X-ray ptychographic imaging	In this tutorial, we are going learn how to design and perform ptychography experiments using high-energy X-rays. Such an emerging technique in synchrotron facilities uses the coherence of the X-ray beam and can provide four information from the same experiment: the absorption and phase-contrast image of the sample and the amplitude and phase of the beam used to scan the sample. Its high-sensitivity to the electron density of the sample makes this technique extremely quantitative. Therefore, we will also learn how to extract quantitative information from the reconstructed images like the refractive index, electron density and mass density of the sample. The experiments will be performed at ID16A and in high vacuum.
id17	A. Bravin, A. Mittone	High resolution micro-CT images of biomedical samples	After a brief description of the setup, we will review with the students the critical parameters for the image quality with practical examples: energy, sample to detector distance, correct alignment of the rotation stage with the optics. We will then acquire some stages of samples of biological interest, and, using local software, we will guide the students in the finding of the rotation center and in the image reconstruction. We will then ask the students to recognize the sample hidden in the non-transparent plastic containers.
id21	H. Castillo Michel, A.E. Pradas	MicroXRF and microXANES for localization and speciation of Ag NPs in environmental samples	We will use the scanning X-ray microscope at ID21 to perform XRF mapping and X-ray absorption spectroscopy at the sub-micron scale on waste water treatment plant sludge before and after incineration, and in plant roots grown in sludge amended soil. The objective is to detect and map the distribution of Ag in the environmental samples and monitor the chemical transformations that they undergo.

Tutorials

Thursday 18 May 2017

Participants in the HSC19 courses will be picked up at 08:45am and 12:45pm & 03:30pm for morning and afternoon sessions respectively from the ESRF entrance hall and accompanied to the appropriate place.

Tutorials	Meeting rooms	Title
V. Favre-Nicolin	BEL 1-01	Coherent X-ray imaging (CDI, Ptychography) reconstruction
R. Mokso	CB 500-501	4D quantification of foams and lungs
J. Vicente	SB 213 (AM) / SB 125 (PM)	3D Geometrical characterisation of porous media with iMorph
A. Mohammad-Djafari	CO 1-10 (AM) / CTRM (PM)	Bayesian Inference and Algorithms for Large Scale Computed Tomography
W. de Nolf	MD-1-21	X-ray powder diffraction imaging
M. Langer	18.1.1 (AM) / CB 337 (PM)	In-line phase tomography at the ESRF
W. Ludwig	ID11 computer room	Reconstruction of 3D grain structures by means of X-ray diffraction contrast tomography
E. Andò	CB 248a	Crash course in particle separation for discrete analysis

Practical and Tutorial Schedule

		Practicals		Tutorials		
Name	First Name	Morning	Afternoon	8:45-11:45	12:45-15:00	15:30-17:45
BORISOVA	Elena	id06	id01	Mokso	Djafari	Langer
BROMBAL	Luca	id17	id16a	Vicente	Langer	Ludwig
COLOMBO	Alessandro	id01	id06	Favre-Nicolin	Ludwig	Mokso
DE PAUW	Ella	id06	bm05	De Nolf	Andò	Vicente
DEHLINGER	Aurelie	id17	id16a	De Nolf	Andò	Djafari
DONATO	Sandro	id17	id01	Mokso	Vicente	Djafari
GIRARD	Gaetan	id06	bm05	Langer	De Nolf	Ludwig
HRIVNAK	Stanislav	id01	id21	Ludwig	De Nolf	Vicente
KAMM	Paul Hans	id06	id01	Mokso	Vicente	Djafari
KANDULA	Neelima	bm05	id06	Vicente	Ludwig	Andò
LANZAFAME	Gabriele Natale	id21	id17	Djafari	Vicente	Andò
LIN	Bi-Hsuan	id21	id16a	Favre-Nicolin	De Nolf	Mokso
LUTZ BUENO	Viviane	id16a	bm05	Ludwig	Mokso	Vicente
MALDANIS CERQUEIRA PERES	Lara	bm05	id16a	Vicente	Andò	De Nolf
MATRAS	Dorota	id21	id06	De Nolf	Mokso	Andò
PACILE'	Serena	id17	id06	Langer	Djafari	Mokso
REDFORD	Sophie	bm05	id21	Djafari	Mokso	Langer
SOLTAU	Jakob	id01	id21	Djafari	Vicente	Langer
THIEDE	Tobias	id16a	id01	Andò	Langer	Mokso
VAMVAKEROS	Antonios	id16a	bm05	Ludwig	Djafari	De Nolf
WITTIG	Nina	id21	id17	Favre-Nicolin	Mokso	Andò
ZDORA	Marie- Christine	id16a	id17	Langer	Ludwig	Djafari
ZHENG	Yi	bm05	id17	Andò	Langer	Ludwig
ZIESCHE	Ralf	id01	id21	Andò	Ludwig	De Nolf

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Poster abstracts

First 3D Tomographic Images of Breast Specimens with Synchrotron Radiation at Elettra

L. Brombal

Department of Physics, University of Trieste and INFN, Aera di Ricerca, Padriciano 99, 34100 Trieste, Italy,
luca.brombal@ts.infn.it

Breast cancer is one of the most frequently diagnosed cancer and still one of the main causes of death for women worldwide. An early detection of the disease is crucial for early intervention, thus providing a significant improvement in the survival rate of the patients. In this context, Breast Computed Tomography (BCT) could be a powerful diagnostic tool and many research groups are working on prototypes and clinical trials [1]. The purpose of SYRMA-3D (SYnchrotron Radiation MAMmography-3D) collaboration is to perform the world's first clinical trial of phase-contrast BCT with Synchrotron Radiation (SR) [2]. If compared with conventional x-ray tubes, SR has a high degree of coherence producing detectable phase effects. Moreover, due to the beam monochromaticity, the reconstructed images are intrinsically free from beam-hardening effects. The imaging device is a single-photon-counting CdTe detector (PIXIRAD-8) with a 60 μ m pixel. The projections first undergo a detector-specific pre-processing, then a 2D phase-retrieval filter is applied and subsequently the tomographic image is obtained using a filtered back projection algorithm. Recently, promising results have been obtained and the first 3D tomographic reconstruction of a breast specimen was performed. Fig. 1 shows two views of the reconstructed sample: the distinction between glandular (bright) and adipose (grey) tissue is clearly visible and the glandular structures are well resolved. In the next future we plan to image several biologic tissues quantitatively evaluating the image quality and optimizing the reconstruction parameters and filters.

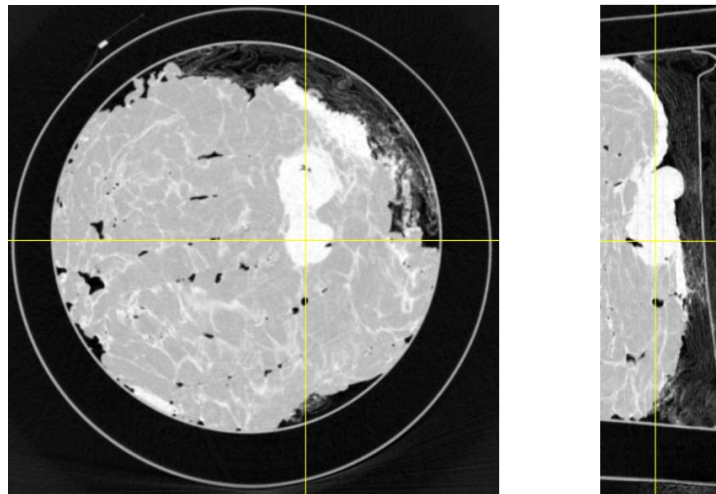


Figure 1: 3D reconstruction of a breast specimen (diameter 9 cm, thickness 3 cm).
Left: axial view. Right: lateral view. Phase retrieval has been applied.

References

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Memetic Phase Retrieval for Coherent Diffraction Imaging

A. Colombo

Università degli Studi di Milano, Via Giovanni Celoria, 16, 20133 Milano, Italy,
alessandro.colombo6@unimi.it

Coherent Diffraction Imaging (CDI) [1] is a lensless technique that allows imaging of matter at a spatial resolution not limited by lens aberrations. This technique exploits the measured diffraction pattern of a coherent beam scattered by periodic and non-periodic objects to retrieve spatial information. The diffracted intensity, for weak-scattering objects, is proportional to the modulus of the Fourier Transform of the object scattering function. Any phase information, needed to retrieve its scattering function, has to be retrieved by means of suitable algorithms, whose performances often represent a handicap for an effective imaging of the sample under study [2].

We present a methodology able to exploit existing approaches, based on an iterative imposition of the constraints, by mixing the information provided by parallel retrieval process with a genetic algorithm [3]. This hybrid stochastic-deterministic approach is, in fact, a memetic algorithm [4] applied to the phase retrieval problem and has been called Memetic Phase Retrieval (MPR) [5].

The performance of MPR has been tested on simulated CDI data, both real-valued and complex-valued, showing performances significantly better than existing approaches.

MPR has been successfully applied to Electron Diffraction Imaging (EDI) and X-Ray CDI data.

A comprehensive description of MPR approach is shown, accompanied by a comparison of its performance with the most known phase retrieval algorithms.

Results on experimental EDI data of nanocrystals are presented, revealing the ability of imaging matter beyond the atomic resolution. Also preeliminary results of X-CDI data are shown, imaging Helium droplets in a pump-and-probe experiment with a X-Ray Free Electron Laser.

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Laboratory X-ray Microscopy and Tomography in the Water Window

A. Dehlinger

Technische Universität Berlin, Institut für Optik und Atomare Physik, Hardenbergstr. 36, 10623 Berlin, Germany, aurehlinger@hotmail.de

In microscopy, where the theoretical resolution limit depends on the wavelength of the probing light, radiation in the soft X-ray regime can be used to analyze samples that cannot be resolved with visible light microscopes on one hand and without extensive sample preparation (as required for transmission electron microscopy). The main advantage of water window X-ray microscopy lies in the large penetration depth and high natural contrast between carbon-based structures (e.g. proteins) and water, which is an ideal condition for the tomographic investigation of biological samples. Soft X-ray microscopes are commonly employed in synchrotron facilities, which constitute tunable and brilliant X-ray sources [1]. However, the required radiation can also be provided by a laser produced plasma source, allowing the establishment of this technology in the laboratory and therefore making it available to a wider scientific community [2].

We present a Laboratory Transmission X-ray Microscope (LTXM) at the Berlin Laboratory for innovative X-ray technologies (BLiX) with a probing radiation energy of 500 eV, provided by a laser-based nitrogen plasma source. Images can be recorded with resolutions of up to 30 nm and within less than one minute. Therefore, samples (e.g. diatoms, living cells or proteins) can be recorded under several projection angles between $+60^\circ$ and -60° , allowing a three-dimensional reconstruction of the sample, which is the key to a more precise and global analysis in various fields of life science.

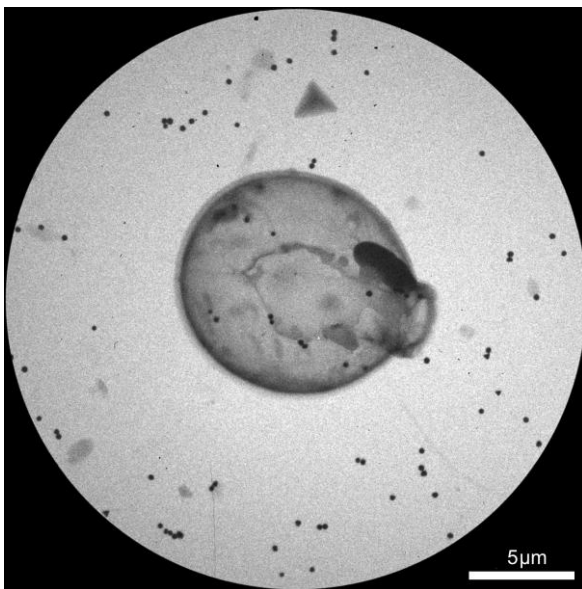


Figure 1: Two-dimensional projection of a diatom with 250 nm gold nanoparticles used for the tomographic reconstruction (magnification: 700x)

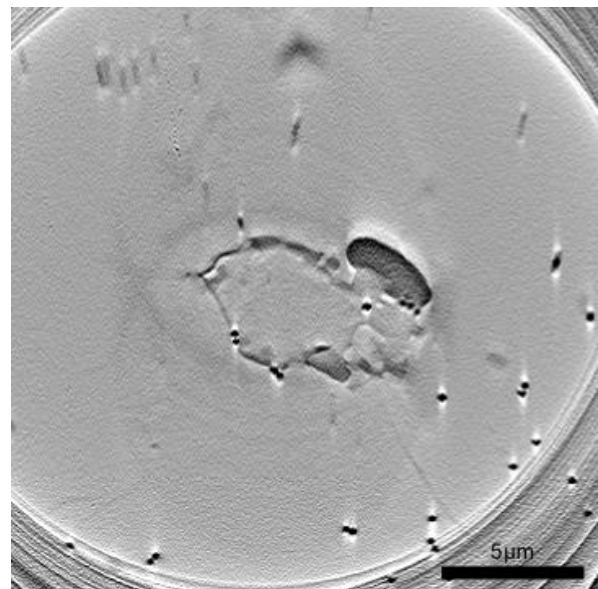


Figure 2: Tomographic reconstruction of a section of the diatom presented in Figure 1

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X-ray Fluorescence and X-ray Absorption Spectroscopic Analysis of Chinese Porcelain dating from the Ming Dynasty

E. De Pauw, E. Verhaeven, P. Tack, S. Bauters, B. Vekemans, L. Vincze
Ghent University, Krijgslaan 281 S12, 9000 Ghent, Belgium, ella.depauw@ugent.be

The oldest findings of Chinese porcelain date back to the Han dynasty, between 206 BC and 220 AD, contributing to more than 2000 years of porcelain history [1]. Until now, the dating procedure of archaeological porcelain samples, was mainly performed via an art-historical approach, differentiating based on the different likes and dislikes of the various emperors, yielding specific styles of porcelain for different eras in the Chinese history. Although this method serves its purpose, a more accurate dating procedure is now available, consisting of quantitative measurements and the determination of (trace) elemental distributions and fingerprints within the different regions of interest of the porcelain fragments.

In our study, two groups of blue and white porcelain samples were investigated using X-ray fluorescence (XRF) spectroscopy; the first group (A) consists of ten shards found in a shipwreck before the Malaysian coasts and a second group (B), of a shard from a plate belonging to a private collection. Via art-historical analyses, both groups determined as kraakporcelain (i.e. porcelain destined for trade to Europe) originating from the Ming dynasty. Additionally, X-ray absorption spectroscopy (XAS) was performed upon the blue pigment in the porcelain shards, confirming its identity as 'Cobalt Blue'. Furthermore, various differences or similarities between the shards were detected. Taking into account that all samples date from the same time period (confirmed by the art-historical analyses), the method shows potential to determine if the porcelain shards were manufactured in the same kiln, or at different locations in China.

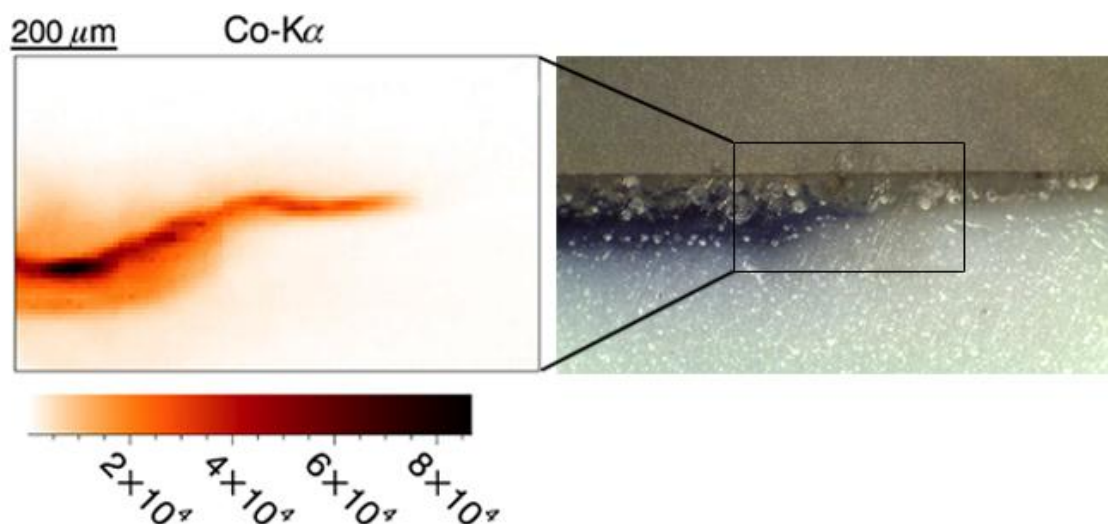


Figure 2: left: X-ray fluorescent map showing the Co distribution within a porcelain shard. Right: optical microscopy image of the shard, with the corresponding area indicated. The different layers present in the porcelain can also be observed, i.e. the white Si body, a blue pigment layer and a transparent glaze layer on top.

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X-ray Micro Computed Tomography with White Synchrotron Beam

S. Donato

Department of Physics, University of Trieste and INFN, Via Valerio 2, 34127 Trieste, Italy,
sandro.donato@fis.unical

The white beam station at the SYEMEP beamline in Elettra is designed to achieve high resolution images or fast scans for microCT. Using a polychromatic spectrum (8-40 keV and high flux) and a 16-bit sCMOS detector, coupled with a high numerical aperture optic, is it possible to obtain images with pixelsize tunable from 1 to 6 μm . This setup allows to study samples where detection of small features is needed but the resulting field of view (compared to the monochromatic setup) is small. Considering the energy spectrum, this setup is primary intended for low and medium absorbing and small specimens.

This work is an overview of some experiments done in the SYRMEP white beam configuration mode applied to biology, geology and material science, and then results obtained with image processing techniques will be shown. Those works come from the scientific collaboration between external users and the staff of SYRMEP and will result in scientific publications already in press [1] or under preparation.

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High Resolution Imaging of Strained Semiconductor Nanostructures

G. Girard

ESRF, 71 avenue des Martyrs, 38000 Grenoble, France, gaetan.girard@esrf.fr

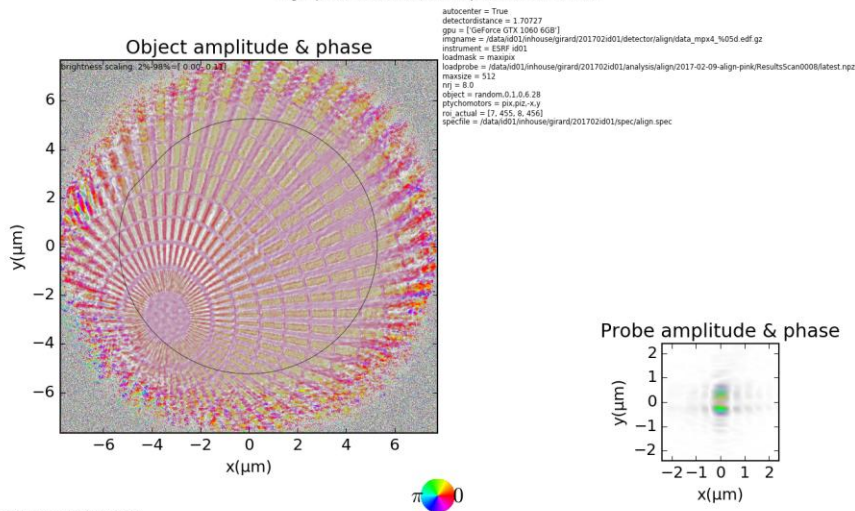
In the scope of X-ray coherent diffraction imaging investigations, notably methodological developments of Bragg CDI techniques, an essential application is the study of strained semiconductor nanostructures and heterostructures [1].

Active devices dimensions have been continuously decreasing (since their efficiency is greatly improved by optical or quantum confinements), and in the same time performance of individual nano-objects has become more sensitive to small variations of structural properties such as shape, strain, defects..., therefore a need has arisen for accurate characterization of individual objects.

X-ray coherent diffraction imaging (CDI) has been developed for the past 15 years, and has been successfully used to reconstruct 2D and 3D nano-objects, including inhomogeneous strain fields using the Bragg geometry [2]. However, reconstruction of nanocrystalline objects using Bragg CDI is a rather complex technique, which has been successful only on a subset of samples like isolated nanocrystals/wires and epilayers, but remains challenging for other types of samples. Further development of these techniques is required to make them more accessible to a wider range of applications and community of users.

As well as the use of Ptychography, an efficient and robust technique which allows recovering both the object and the X-ray probe, the scanning probe technique developed at ID01 beamline (ESRF, Grenoble) can yield unique strain mapping [3] that has been experimented on SiGe nanostructures grown on silicon oxide with a silicon substrate.

Scan #11, 1025 frames, pixelsize= 10.7nm, LLK= 12.965
algo=probe=1,100AP,100ML,nbprobe=3,200AP,50ML



PtyNX v2.7.0, finished at 2017/03/17 16:26:53

Figure 2: Object and probe reconstruction from a ptychography measurement on ID01 beamline

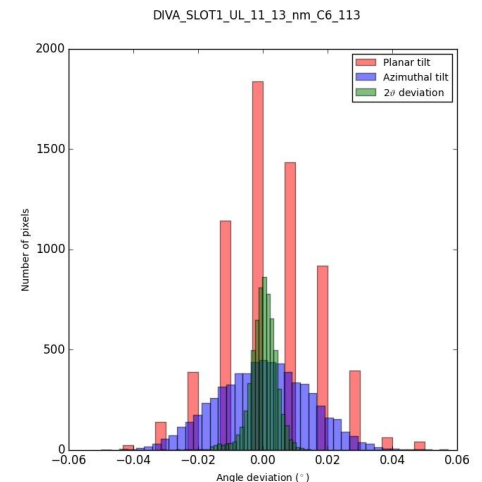


Figure 1: Histogram of the tilts of the crystalline lattice, in-plane, out-of-plane, and 2θ deviation for a 12 nm-thick SiGe layer grown on silicon oxide at CEA-LETI

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3D Tomographic Imaging of Biological Objects using Hard X-ray Bragg Magnifier Microscope

S. Hrivňak¹, J. Uličný¹, L. Mikeš^{1,2}, A. Hovan¹ and P. Vagovič^{3,4}

¹Center for Multimodal Imaging (CMI), Department of Biophysics, Institute of Physics, Faculty of Science, P. J. Šafárik University, Jesenná 5, 04154 Košice, Slovakia, ²Department of Computer Science, Faculty of Science, P. J. Šafárik University, Jesenná 5, 04154 Košice, Slovakia, ³European XFEL, Albert Einstein Ring 19, 22761 Hamburg, Germany, ⁴Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany, stanislav.hrivnak@student.upjs.sk

We present an alternative method for 3D tomographic imaging of microscopic biological objects in hard X-ray regime, based on Bragg Magnifier (BM) principle [1]. BM microscope uses asymmetrically cut Germanium crystals to magnify X-ray beam with advantages such as shorter propagation distances and increased dose efficiency, while achieving decent spatial resolution. This work focuses on the 3D reconstruction method to interpret the X-ray tomographic holograms using single-distance phase retrieval algorithm developed specifically for Bragg Magnifier, which is followed by filtered back-projection. We use a modification of contrast transfer function approaches developed for propagation based phase-contrast imaging and in combination with iterative constraint-based phase retrieval algorithm [2] we obtained faster and more robust reconstruction method. Our algorithm was successfully applied to both synthetic and real-world experimentally measured holograms as demonstrated on 3D electron density reconstruction of model organism Tardigrade (Fig. 1). We reached isotropic spatial resolution 300 nm approaching theoretical resolution limit for the given experimental setup.

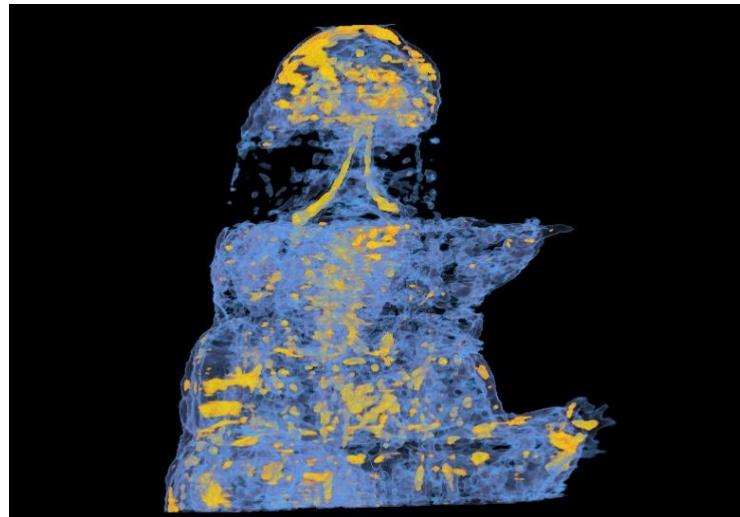


Figure 1: 3D reconstruction of model organism Tardigrade after segmentation. Small yellow parts correspond to the cell nuclei.

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Fast Synchrotron X-ray Tomography of Dynamic Processes in Aluminium Alloy Foams

P.H. Kamm^{1,2}, F. García-Moreno^{1,2}, T.R. Neu², R. Mokso³ and J. Banhart^{1,2}
¹Applied Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, ²Institute for Materials Science and Technology, Berlin Institute of Technology, Germany, ³MAX IV Laboratory, Lund University, Sweden, paul.kamm@helmholtz-berlin.de

The improvement of metal foams requires a deeper understanding of the fundamental mechanisms that act during foaming. X-ray tomography provides the 3D information needed to reveal the structural complexity of foams, but only recently temporal resolutions have become available that are sufficient to capture foam dynamics as well.

Series of fast synchrotron X-ray tomographies, performed at the Tomcat beamline of the Swiss Light Source synchrotron facilities, were taken continuously at a sub-second temporal resolution while aluminium alloy precursors were foamed with a laser based heating device in an X-ray transparent setup for several minutes [1]. The entire foaming process from the solid precursor to the expanded liquid foam was captured and the gas nucleation and bubble growth were analysed.

The quantitative analysis of the obtained four dimensional data has been performed in terms of the evolution of pore number, size distribution and shape development. Coalescence as well as coarsening of bubbles has been observed and bubble shape evolution has been followed revealing a deeper insight into the nucleation process [2].

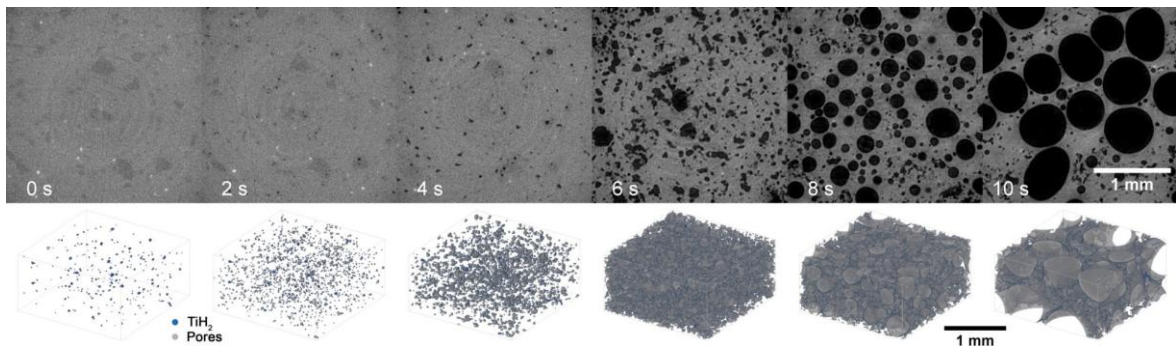


Figure 1: Tomographic slices (top) and 3D renderings (bottom) of pores (grey) and blowing agent particles (blue) of the early foaming stage of an AlSi8Mg4 alloy for different times

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The Route to shear Failure in a Non-Porous Rock Revealed X-ray Micro Tomography

N. Kandula¹, F. Renard¹, J. Weiss³, D.K. Dysthe², B. Cordonnie^{1,4} & M. Kobchenko¹

¹Departments of Geosciences, University of Oslo, Norway, ²Departments of Physics, University of Oslo, Norway, ³ISTerre, Universite´ Grenoble Alpes and CNRS, CS40700, Grenoble 38058, France, ⁴The European Synchrotron, ESRF, beamline ID19, Grenoble, France, neelima.kandula@geo.uio.no

Microscale heterogeneities guide the mechanism of failure in rocks of Earth's crust. In a non-porous rock these heterogeneities correspond to grains and grain boundaries and provide insights into understanding the mode of failure and existence of precursors. Brittle compressive failure is exhibited by non-porous rocks and in recent years much attention has been given to understand it [1]. We have used a novel experimental technique that couples X-ray microtomography with a unique triaxial deformation apparatus, HADES Figure 1a [2] installed at European Synchrotron Radiation Facility that can simulate in-situ rock deformation under crustal conditions at the laboratory scale. Cylindrical Carrara marble samples of centimetre scale are deformed until failure at room temperature at a varying confining pressure from 20 MPa to 30 MPa. The stress versus strain curve is shown in Figure 1b and is characteristic of a brittle fracture in the quasi-static limit. 3D data (volumes) obtained for every step increase in axial stress were segmented to extract the micro-fractures. Micro crack volume saturates to a value near to zero and increases non-linearly from yield point towards rupture, indicating that precursory signals are present before rupture. Figures 1c-e show the micro crack volumes respectively with increasing stress, figure 1e corresponds to 196 MPa, the onset of failure. The statistical properties of the population of growing cracks is characterized to search for spatial correlations and further the density of cracks towards failure is shown to increase as a power law.

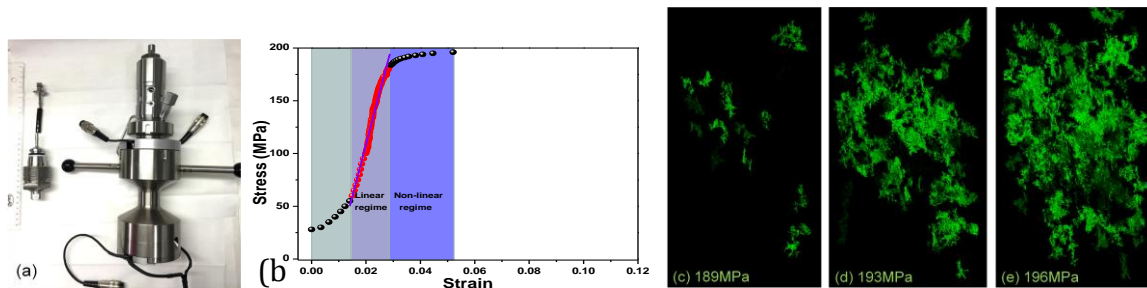


Figure 1: (a) Photograph of the deformation apparatus HADES (body of the rig) used for time-resolved X-ray tomography of failure in rocks. (b) Stress-strain curve for marble sample under triaxial compression at confining pressure of 25 MPa and at room temperature (failure at 197 MPa). Development of micro cracks prior to failure in the sample at (c) 189 MPa, (d) 193 MPa, (e) 196 MPa

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Gas Exsolution and Bubbles Nucleation from the 1669 Lava Flow of Mount Etna (Italy): Evidences from Phase-Contrast Synchrotron X-ray Microtomography

G. Lanzafame^a, C. Ferlito^b, L. Mancini^a, F. Casetta^c

^aElettra-Sincrotrone Trieste S.C.p.A., SS 14, Km 163.5 in Area Science Park, 34149 Basovizza (Trieste), Italy, ^bDipartimento di Scienze Biologiche, Geologiche e Ambientali, Università di Catania, Corso Italia 57, I-95129 Catania, Italy, ^cDipartimento di Fisica e Scienze della Terra, Università di Ferrara, Via Saragat 1, I-40400 Ferrara, Italy, gabriele.lanzafame@elettra.eu, lucia.mancini@elettra.eu

Bubbles are usually present in lavas, increasing in their size and number from bottom to the top of vertical profile of the flows. Their appearance is commonly interpreted as the final stage of the degassing processes starting and massively occurring at depth, before the eruption. We present in this work the results of a detailed study of size, shape and volumetric distribution of bubbles in lavas from one of the most voluminous and destructive historic events of this volcano, the 1669 eruption of Mount Etna (Italy) [1]. The lava flows emitted during this eruption extend up to 18 km from the craters, and are characterized by the massive presence of bubbles even at many kilometres away from the emission point. This is in contrast with the models predicting an almost total exsolution of magmatic gases before the eruption, at depth of several kilometres beneath the volcano edifice. Sampling of the 1669 lava field has been performed along the longitudinal profile of the field at increasing distance from the vent. Rocks have been analysed by X-ray fluorescence and phase-contrast synchrotron X-ray computed microtomography in order to extract three-dimensional (3D) qualitative and quantitative information on the bubbles network. The use of synchrotron light allowed to investigate the samples at high spatial and contrast resolution. Image analysis by Pore3D software library [2] allowed to retrieve the 3D morphology and distribution of the micro-bubbles present in the lava, avoiding the limitations of the classic 2D analysis on thin sections. Results indicate that bubbles in lavas are present in various amount, up to 18% of the rocks volume, and are randomly distributed, with no regards for the distance from the vent. Their casual abundance, spatial distribution and morphological characteristics indicate large nucleation from syn- to post-eruptive stage, during the lava flowing and probably after it halted its run. These observations are in contrast with the general view that considers the magma largely degassed and the volcanic gas species (mostly H₂O) as largely exsolved when magma is erupted. Our results indicate that the exsolution of bubble-forming volcanic gases can occur far from the emission vent and right before the complete solidification of the lava. Finally, this process could easily explain, for the case of 1669 eruption, the impressive fluidity of the lavas, which display pahoehoe morphology 16 km away from the emission vent.

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The Progress and Capabilities of the X-ray Excited Optical Luminescence at X-ray Nanoprobe at Taiwan Photon Source

B.-H. Lin, H.-Y. Chen, S.-C. Tseng, J.-X. Wu, B.-Y. Chen, C.-Y. Lee, S.-H. Chang,
G.-C. Yin, M.-T. Tang

National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu,
Taiwan, bihsuan@nsrrc.org.tw

X-ray excited optical luminescence (XEOL) and time-resolved XEOL as well as the 40nm spatial resolution which is focused by Montel KB mirrors are developed in the X-ray nanoprobe beamline at the new synchrotron facility, Taiwan Photon Source (TPS). Photoluminescence (PL) is one of the efficient and fundamental tools for characterising the optical properties of the wide band gap semiconductor materials. The advantages of using synchrotron radiation as the excitation source are that the tuneable X-ray energy allows the preferential excitation of the elements through the X-ray absorption edges, and a suitable time structure of the synchrotron can be used to study the dynamics of luminescence of the materials. Before the nanoprobe beamline constructing completion, the XEOL experiment was measured by unfocused X-ray beam at Taiwan Light Source (TLS). In this study, by means of XEOL to study the optical properties of O and Zn polarity of c-plane ZnO bulks has been achieved successfully. The low temperature (less than 5K) and temperature-dependent XEOL with X-ray excited energy below, at and above the Zn K-edge (9.659keV) were used to obtain the further information of the optical mechanisms of the two polar faces. The first excited state ($n=2$) of A free exciton was observed at 3.422eV with only for O-polar. The result indicates that O-polar has higher optical quality than Zn-polar. The exciton-phonon (A_1 -LO) coupling strength will be changed by using different X-ray excitation energy while the temperature above 150K. The current design of the nanoprobe beamline and the detail XEOL experimental results will be reported.

Scanning-SAXS Microscopy: Higher Dimensionality, Information Level and Reconstruction Complexity

V. Lutz-Bueno^{*}, M. Guizar-Sicairos^{*}, A. Diaz^{*}, J. Kohlbrecher^{**}, O. Bunk^{*} and A. Menzel^{*}

^{*}Swiss Light Source, Laboratory for Macromolecules and Bio-imaging and ^{**} Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen, Switzerland, viviane.lutz-bueno@psi.ch

Nature builds materials with excellent mechanical properties from weak building blocks. This hierarchical structuring is applied successfully in materials science for artificial and bio-mimetic materials. Visual analysis of such samples through microscopy is fundamental to discover relationships between structure, shape and function of multiphase hierarchical materials. A recurrent limitation of microscopy is the poor differentiation, identification and quantification of phases and building blocks without contrast enhancement of a non-destructive sample. The lack of methodology to automatically classify and quantify sample composition and its phase distribution hinders the understanding and tuning of structure-property relationships. The signal of small-angle X-ray scattering SAXS comes from the interaction of matter with light, as a signal sensitive to the sample's electronic composition and structure, covering the ideal length scale to probe hierarchical materials. In this poster we will show the development of microscopy and tomography scanning-SAXS methods for automated phase identification, segmentation and quantification. The recent improvements in synchrotron brilliance, detector resolution and data science are part of our "toolbox", especially for data collected in scanning mode, which usually requires a compromise between resolution and sample size. Assuring that such a method is available to the scientific community, especially at synchrotrons where selected users perform state-of-the-art research, is the obvious path to accelerate materials science.

Unveiling Fossil Microbial Life with Multi-Scale Imaging Techniques

L. Maldanis^{1,2}, D. Galante¹

¹Brazilian Synchrotron Light Laboratory, R. Giuseppe Maximo Scolfaro 1000 Campinas-SP Brazil

²IPANEMA Research Platform, Synchrotron Soleil, L'Orme des Merisiers, Saint-Aubin, France,

lara.maldanis@lnls.br

Microfossils are morphological biosignatures of microorganisms preserved in the geological record and comprise the oldest direct record of life on Earth. Their study can provide information about the palaeoenvironment and the origin and evolution of life on the planet[1]. However, due to the high level of geological processing over billions of years, the micrometric size and the chemical composition (highly dense and homogeneous rocks), the study of such structures has been limited, and many questions about their morphology, preservation and biogenicity remain unsolved[2,3]. The use of micro-analytical imaging techniques based on different physical phenomena has been proposed as a potential approach to overcome these limitations, exploring both the morphology and chemical composition of the samples in its geological and paleoenvironmental context.

Here we present some challenges of using X-ray imaging to study microfossils, and also some preliminary results of micro-Raman, Confocal Laser Scanning Microscopy and micro-CT analysis of Brazilian Permian microfossils. Through complementary data, these techniques allowed the identification of in situ structures with a non-destructive approach, the evaluation of 3D distribution of carbonaceous organic matter, and also provided information about geochemical maturation of the preserved specimens. The use of other X ray imaging techniques, as phase contrast micro-CT, Ptychography, micro-XRF and micro-XAS are also proposed as next steps to potentially assess fundamental aspects of subcellular morphology correlating with chemical composition. Together, these approaches can largely contribute for establishing more robust biogenicity criteria, helping to understand ancient life, refine taxonomic data and cladistics, and also helping to recreate more accurately paleoecological and paleoenvironmental scenarios.

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X-ray Diffraction Computed Tomography - Data Collection Strategy and Application for Operando Studies of Catalytic Systems

D. Matras

School of Materials, University of Manchester, Manchester, Lancashire M13 9PL, UK, Research Complex at Harwell, Harwell, Didcot, Oxon, OX11 0FA, UK, matras.dorota@gmail.com

X-ray diffraction computed tomography is a technique that combines powder X-ray diffraction (PXRD) with computed tomography (CT). In contrast to standard computed tomography (CT), based on the difference in the attenuation of X-rays from the materials present in the sample, XRD-CT uses the difference in the diffraction signals from the crystalline materials present in the sample. Therefore, additional physico-chemical information is obtained. In the reconstructed image, each pixel corresponds to a complete diffraction pattern, and thus different crystalline chemical species can be mapped inside the cross section of a bulk object [1].

XRD-CT technique is applied in synchrotrons (ID15 of ESRF), due to its remarkable properties (high flux, monochromatic beam, state-of-the-art detector, etc.) and was found to be a suitable technique for the *in situ* studies of heterogeneous catalysts, providing high temporal and spatial resolved data [2]. The ultimate goal of catalysis is to understand the relation between catalyst structure and its function in the studied reaction. For this purpose, it is important to observe the behaviour of the catalyst under *operando* conditions, collecting the information at different length scale over the entire volume of catalyst [3]. Recently, a new data collection strategy called interlaced XRD-CT was developed [4] in order to provide the post experiment choice between temporal and spatial resolution. Another data collection strategy, allowing us to image the whole catalyst bed (cross section by cross section) in a reasonable amount of time is being developed.

The purpose of this work is to demonstrate how the XRD-CT technique works together with the recent development of data collection strategy that is necessary for the *in situ* studies of materials. Different types of data that can be obtained with this technique are presented, with the example of catalyst for the OCM (oxidative coupling of methane) process.



Acknowledgement

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Image Quality Analysis in Propagation-Based Phase-Contrast Breast CT

S. Pacilè

Elettra, Sincrotrone Trieste, SS 14 KM 163-5, Area Science Park, Basovizza, 34012 Trieste, Italy and Department of Engineering and Architecture, University of Trieste, Trieste, Italy, serena.pacile@elettra.eu

In the framework of breast imaging, in contrast to mammography, commonly used to diagnose breast cancer, novel three-dimensional X-ray based imaging technologies, such as Digital Breast Tomosynthesis and breast-dedicated Computed tomography eliminate the problem of overlying tissues in conventional 2D images [1,2]. Thus, they significantly improved the efficiency of large scale screening programs. Despite that, the small difference in X-ray attenuation, in particular between the glandular and tumour tissue, still constitutes a major problem in these methods [3]. In recent years, the development of X-ray phase-contrast imaging techniques, which are able to measure the effects of X-rays refraction in the body, have shown promising results for refining breast cancer diagnosis. These techniques permit the visualization of soft-tissue structures that are not detectable by use of conventional X-ray radiographic methods, and also hold the potential to reduce the radiation dose delivered to the patient [4,5,6]. Among the different phase-contrast techniques, the propagation based phase-contrast CT (PB-CT) method is the one analysed in this work. PB-CT does not require the use of any additional X-ray optical element, it is therefore the easiest method to implement.

Up to now the required level of spatial coherence of the incident X-ray beam used in PB-CT has practically limited its application to synchrotron facilities. However, the optimization of PB-CT for breast imaging will provide practical guidelines to evaluate novel generator-based phase-contrast setups (including analyser-based imaging, edge-illumination, and grating-based imaging) or compact sources.

The goal of this work is to evaluate how experimental conditions and reconstruction parameters affect the image quality in breast PB-CT and establish, from a quantitative point of view, the optimal combination of acquisition (distance, energy and detector) and reconstruction ($\delta\beta$ ratio and algorithm) parameters.

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The JUNGFRAU Photon Detector for SwissFEL

S. Redford

Paul Scherrer Institut, 5232 Villigen PSI, Switzerland, sophie.redford@psi.ch

The JUNGFRAU detector is a charge-integrating hybrid silicon pixel detector developed at PSI for photon science applications, in particular for the upcoming free electron laser SwissFEL. With a high dynamic range, analogue readout, low noise and three automatically switching gains, JUNGFRAU promises excellent performance not only at XFELs but also at synchrotrons in areas such as protein crystallography, ptychography, pump-probe and time resolved measurements [1]. To achieve its full potential, the detector must be calibrated on a pixel-by-pixel basis.

This contribution will introduce the JUNGFRAU detector and present the current status of the calibration project, in which a variety of input charge sources are used to parametrise the energy-response of the detector across four orders of magnitude of dynamic range. Building on preliminary studies [2], the first full calibration procedure of a JUNGFRAU 0.5 Mpixel module will be described. This three-step method uses fluorescence measurements for an absolute calibration of high gain, followed by backplane pulsing [3] and an internal current source to extend the calibration to medium and low gains. Calibrated modules have already been used in proof-of-principle style PX and ptychography experiments at the SLS. A first look at these results will be shown.

The calibration is validated using alternative sources of charge deposition, including direct X-ray tube beam illumination and measurements from test beam campaigns at ESRF, LCLS and the SLS. The findings from these measurements will be presented. Aspects such as the conversion of charge to number of photons, treatment of double-size pixels, constraints between individual gain calibrations and the origin of non-linear response will also be discussed.

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Imaging with Hard X-rays and Nanometer Resolution using Multilayer Zone Plates (MZP)

J. Soltau, Ch. Eberl, H.-U. Krebs and M. Osterhoff

Institute for X-ray Physics, University of Goettingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany,
 jakob.soltau@uni-goettingen.de

The advantage of hard X-ray microscopes is their ability to perform non-invasive photonic imaging without the requirement of a vacuum. The resolution of microscopes operating in the hard X-ray energy range is currently limited by the numerical aperture of the setup given by the radiation source and the X-ray optics.

X-ray microscopes operating in the soft X-ray energy range often use zone plates as optics. The resolution of zone plates in general is determined by their smallest zone width. The challenge in fabricating zone plates for the hard X-ray energy range is the high aspect ratio, defined by the large optical thickness ($> 1 \mu\text{m}$) - needed due to the low interaction between photons and matter - and the already mentioned small zone widths (down to 5 nm).

The technique of pulsed laser deposition enables the fabrication of zone plates - the so called multilayer zone plates (MZP) - with zone widths of only 5 nm and an optical thickness up to $30 \mu\text{m}$ (see fig. 1a and fig. 1b). This promises imaging at nanometer resolution in a hard X-ray microscope setup [1].

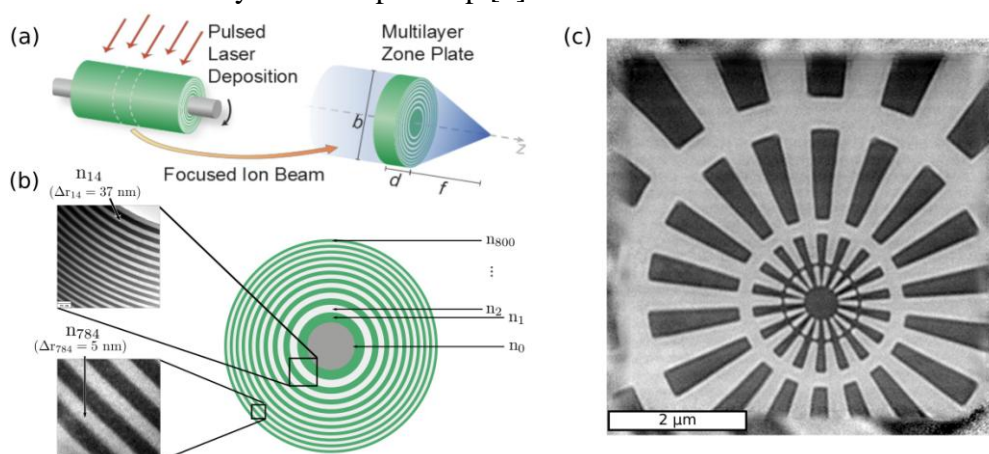


Figure 1: (a) Sketch of the pulsed laser deposition (PLD) process to fabricate the MZPs. (b) Illustration of an MZP together with electron microscope images of the individual zones at different radii with zone widths down to 5 nm. (c) Scanning X-ray microscope image of a Siemens star with smallest feature size of 50 nm. Taken with the new high-resolution setup at the P10/Petra III/DESY using a MZP at 13.8 keV

Latest experiments using MZPs at synchrotrons demonstrated successfully a resolution of a few nanometers in a wide X-ray energy range from 8 keV at DESY/Petra III and for the first time with photon energies above 100 keV at ESRF. Exemplary data of the most recent beam time is shown in Figure 1c. In a scanning microscope setup a Siemens star was imaged at a photon energy of 13.8 keV using a MZP with 800 zones and an outermost zone width of only 5 nm. The smallest features of the star have a width of only 50 nm and are clearly resolved with the new vibration reduced high-resolution setup at Petra III/P10.

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Residual Stress Analysis in Selective Laser Melted Parts of Superalloy 718

T. Thiede

Bundesanstalt für Materialforschung und -prüfung (BAM), Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin, Germany, tobias.thiede@bam.de

Additive Manufacturing (AM) by Selective Laser Melting (SLM) offers ample scope for producing geometrically complex parts in comparison to the traditional subtractive manufacturing strategies. Developing during the manufacturing process, residual stresses may limit the application of SLM parts by reducing the load bearing capacity as well as induce unwanted distortion depending on the boundary conditions specified in manufacturing.

The present study aims to evaluate the bulk residual stresses in SLM parts by using neutron diffraction measurements performed at E3 line -BER II neutron reactor- of Helmholtz-Zentrum für Materialien und Energie (HZB) Berlin. Together with microstructure characterization and distortion measurements, it is possible to describe the stress state throughout the whole sample. The sample was measured in as-build condition (on a build plate) and after releasing from the build plate. The used material is the nickel based superalloy 718. This alloy is widely used in aerospace and chemical industries due to its superior corrosion and heat resistant properties.

Obtained results indicated different residual stress states for each of the transversal, longitudinal and normal component. The normal and transversal component exhibits a rather compressive behavior while the longitudinal was tensile in the center part of the sample and became compressive towards the tip. As expected, the absolute values of all stress components decreased after releasing the sample from the building plate. A surface scan utilizing a coordinate-measuring machine (CMM) allowed us to present top surface distortion before and after releasing. The top surface showed a distortion around $\pm 80\mu\text{m}$ after releasing. Microstructure evolution in the scanning-building cross-section is largely dominated by columnar grains. In addition, many small random orientated grains are prominent in the regions of a laser overlap during SLM.

In summary, for the sample of superalloy 718 manufactured by SLM, a small distortion occurred when removing the sample from the build plate whereby the residual stress state decreases. Moreover, the observed columnar grains in the building direction could give a reason for the lowest stress values in that normal direction. However, the most important parameter controlling the residual stresses is the temperature gradient. Hence, future investigations are planned for a different scan strategy to distribute the laser impact in a more homogenous manner.

Unravelling the Chemical Evolution of Catalytic Materials under Operating Conditions with Real Time Chemical Imaging

A. Vamvakeros^{1,2}, S.D.M. Jacques^{2,3}, V. Middelkoop⁴, M. Di Michiel⁵, A.M. Beale^{1,2*}

¹Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK, ²Research Complex at Harwell, Harwell, Didcot, Oxon, OX11 0FA, UK, ³School of Materials, University of Manchester, Manchester, Lancashire, M13 9PL, UK, ⁴Flemish Institute for Technological Research, VITO NV, Boeretang 200, Mol, Belgium, ⁵ESRF, 6 Rue Jules Horowitz, 38000 Grenoble, France, andrew.beale@ucl.ac.uk

The imaging of catalysts and other functional materials under reaction conditions has advanced significantly in recent years [1]. The combination of the computed tomography approach with X-ray diffraction (XRD-CT) enables local chemical and physical state information to be extracted from within the interiors of intact materials which can be, by accident or design, commonly inhomogeneous. The spatially resolved signals obtained can reveal information that would otherwise be lost in bulk measurement. Studying intact materials rather than idealised powders allows for behaviour under industrially relevant conditions to be observed. We will show here how XRD-CT has been used to track, for the first time, the evolving solid-state chemistry taking place inside a working catalytic membrane reactor used for the oxidative coupling of methane [2]. Furthermore, recent technical advancements in the XRD-CT technique are also reported. More specifically, a new data filtering strategy to remove/suppress artefacts generated in XRD-CT data due to large crystallites present in the sample [3] and a new data collection strategy, introduced as interlaced XRD-CT, which bridges the gap between spatial and temporal resolution of an XRD-CT scan [4], are presented.

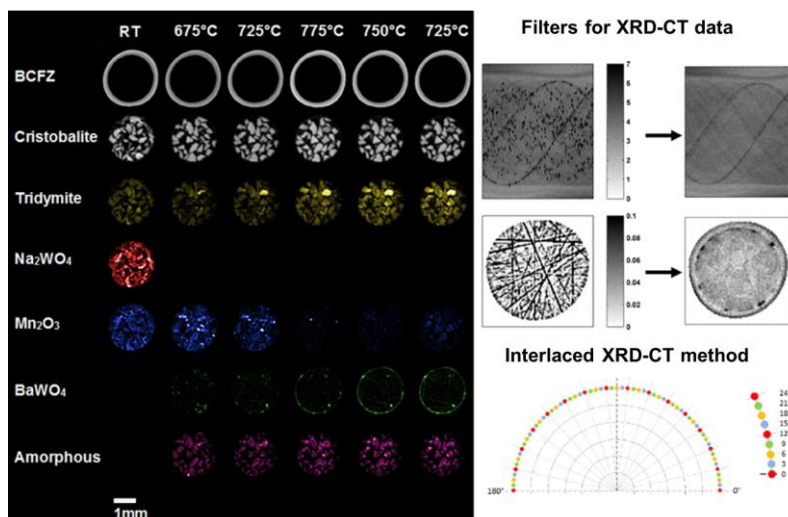


Figure 1: *Left:* Phase distribution maps of a BCFZ – Na-Mn-W/SiO₂ catalytic membrane reactor as determined from XRD-CT data, *Top Right:* Demonstration of the effect of a trimmed mean filter in XRD-CT data, *Bottom Right:* An Interlaced XRD-CT scan consisting of four low spatial/high temporal resolution XRD-CT scans

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Bone Microstructure Revealed by Combined Sub-micron Resolution Diffraction and Fluorescence Tomography

N.K. Wittig, S. Frølich, M.E. Birkebæk, J. Palle, M. Østergaard, K. Spiers, J. Garrevoet, H. Birkedal

Dept. of Chemistry and iNANO, Gustav Wieds Vej 14, 8000 Aarhus C, Denmark, nkw@chem.au.dk

Bone is a complex hierarchical material adapted to withstand applied loads. It has essential structural features ranging from the nanoscale to the macroscopic. The link between bone structure and function, and especially the contribution of the nanoscale structural elements on the macroscopic properties is however still poorly understood. The osteon is an essential building block in human long bones and contributes to highly anisotropic mechanical properties. In this motif, mineralized collagen fibrils are arranged in a twisted plywood structure surrounding a Haversian canal (Figure 1). It has been shown that the indentation modulus varies periodically with the osteon lamellae and that this is positively correlated with the mineral content [1], but exactly how the mineral phase contribute to the mechanical properties of bone remains unanswered. In addition, oligo elements such as Sr play an important role in bone function [2], but how they are incorporated into the bone matrix is not known. Therefore, we have applied combined Diffraction Tomography (DT) and Fluorescence Tomography (FT) at Petra-III, beamline P06 with sub-micron resolution to investigate how the nanocrystalline component and elemental composition varies throughout the osteon. This experiment combines the capabilities of diffraction and fluorescence with those of computed tomography to allow for reconstruction of a diffractogram and a fluorescence spectrum in each volume element within the sample [3]. The resulting >1.5 million diffractograms were Rietveld refined using MultiRef [4] to obtain typical crystallographic parameters, including unit cell parameters, profile parameters etc. This revealed a periodic variation of the crystal properties from the center of the osteon and out as well as highly different elemental make up of osteonal and interstitial bone. In addition we observed altered crystal properties surrounding the cellular network lying buried within the bone matrix, thus providing insight into yet another open question within bone research.

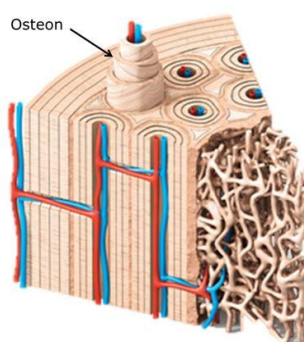


Figure 1: Section of long bone displaying osteons; cylindrical motifs with concentric lamellae surrounding a central (Haversian) canal

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X-ray Phase-Contrast Imaging and Metrology using Periodic and Random Wavefront Modulators

M.-C. Zdora

Diamond Light Source, Didcot, UK & Department of Physics & Astronomy, University College London, Gower Street, WC1E 6BT London, UK, marie-christine.zdora@diamond.ac.uk

In the past years, grating-based [1,2] and more recently speckle-based [3,4] methods have attracted increased interest for X-ray phase-contrast imaging and wavefront sensing. Both techniques rely on the sample-induced modulation of an interference pattern created by a phase modulator (PM), periodic or random, to encode the phase information. Despite the great potential and rapid development of the two techniques, a number of challenges impede their wider use under more difficult conditions, including the requirements of extremely small, equidistant step sizes and the large number of stepping positions.

We here present a technique that overcomes the limitations of grating- and speckle-based imaging in a unified approach [5]. The proposed Unified Modulated Pattern Analysis (UMPA) can be applied to periodic as well as random reference patterns.

The UMPA approach is based on acquiring a few projections with and without the sample in the beam, at different PM positions with step sizes larger than the typical feature size of the reference pattern. The pattern modulated by the sample in the beam can be expressed in terms of the reference pattern without sample, considering the displacement, change in intensity and change in amplitude of the pattern caused by refraction, absorption and small-angle scattering in the specimen. A windowed least-square minimisation between modelled and measured data, summed over the contributions from all measurements, delivers the multimodal image signals. Adjusting the analysis window size and number of PM steps allows tuning of the signal sensitivity with respect to the spatial resolution and scan time.

Figure 1 shows the reconstructed multimodal signals of a small flower bud imaged at Diamond I13-1 with the UMPA method using a piece of random sandpaper as a PM.

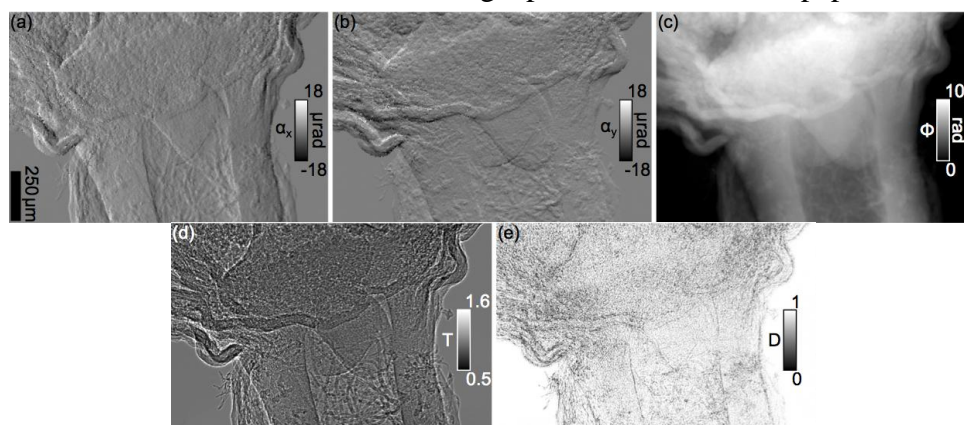


Figure 1: Multimodal images of a small flower bud. (a) Differential phase in the horizontal and (b) vertical directions. (c) Total phase shift integrated from (a) and (b). (d) Transmission signal. (e) Dark-field signal.

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A Micro-CT Study of Barley Germination Process

Y. Zheng and C. Gundlach

Department of Physics, Technical University of Denmark, 2800 Lyngby, Denmark, yizhe@fysik.dtu.dk

The quality of malt is essential for beer production. During malting, the seeds are soaked in water and germinate. During germination, enzymes degrade part of the starch to sugar changing the density of the inner part of the seed. Visualizing this structural change can help to better understand the process of malting. Traditionally, the visualization of the germination process was performed with a 2D light microscopy on slices of barley. It has been proposed that the germination front (where the density decreases) advances parallel to the longitudinal direction of the barley seed [1]. However, the thin slice for light microscopy was usually cut along the longitude direction of the seeds and thus information in the transverse direction may have been overlooked. Micro-CT can provide a full understanding of the direction of the germination front in barley seeds since it is a non-invasive 3D method. In our pilot study with a micro-CT we found that, in contrast to [1], a decrease of density was formed around the crease and quickly expanded along the transverse direction of the barley grain. In conclusions, micro-CT is a promising method to unfold essential information regarding barley seed germination process that cannot be easily discovered in 2D invasive methods.

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Simulation of Flux Trapping Behaviour in Type II Superconductor using Polarised Neutron Imaging

R. Ziesche^{1,2,3}, I. Dhiman^{3,4}, J. Nicol³, L. Riik³ and W. Treimer^{3,5}

¹Department of Chemical Engineering, Univ. College London, Torrington Place, London WC1E 7JE, UK
²STFC, Rutherford Appleton Laboratory, ISIS Facility, Chilton, OX11 0QX, UK, ³Helmholtz Zentrum für Materialien und Energie, FG-GTOMO, 14109 Berlin, Germany, ⁴Chemical and Engineering Materials Div., Oak Ridge National Lab., Oak Ridge, Tennessee 37831, USA, ⁵University of Applied Sciences, Beuth Hochschule f. Technik, FB II, 13353 Berlin, Germany, ralf.ziesche.16@ucl.ac.uk

Superconductor like RRR 300 Nb are standard materials for high-gradient accelerator applications such like superconducting radio-frequency (SRF) systems. These systems are cooled down by liquid helium into the superconducting phase where the electrical resistance drops down to zero. Losses in the rf quality factor Q depend on the surface resistance R_s , which in turn includes a term dependent on trapped flux. [1]. By cooling down Nb cavities into the superconducting phase ($T \leq T_c = 9.2K$) surrounding magnetic fields in the amount of the earth field could be trapped inside the cavity walls and cause Q disease. We studied flux trapping process for a RRR 300 Nb disk sample ($r = 5.0mm$, $h = 4.5mm$) treated with buffered chemical polishing (BCP $\approx 150\mu m$) to investigate how flux of a constant homogeneous external field B_{ext} are trapped inside the superconducting bulk. Polarised neutrons are perfect for quantifying trapped flux inside the bulk of a superconducting sample and the surrounding magnetic stray field, because the neutron spin performs Larmor precessions in the B-field. When the neutron spin interacts with the magnetic field, it begins to make Larmor precession, dependent on the magnetic field strength and the path integral $\int \vec{B} d\vec{s}$ through the sample. This path-dependent neutron spin rotation is used to visualize the magnetic structure. For a better understanding of the experimentally obtained radiographs we correlate the results with simulated theoretical modeled magnetic field distribution. The magnetic stray field can be described by $\vec{H}(\vec{r}) = -\vec{\nabla}\Phi(\vec{r})$ (fig. 1a). Further the magnetic field dependent Larmor spin precession of a polarised neutron beam $\vec{P}(z)$ through the field can be theoretical calculated by semi-classical spin rotation formalism $\frac{d\vec{P}(z)}{dz} = \mathfrak{A}(z) \cdot \vec{P}(z)$ where \mathfrak{A} is the \vec{B} dependent rotation matrix (fig. 1b). [2] [3]

In our study we compared simulated polarised neutron radiographs with experimental obtained trapped flux in RRR 300 Nb (fig. 1c) as a function of temperature and magnetic field.

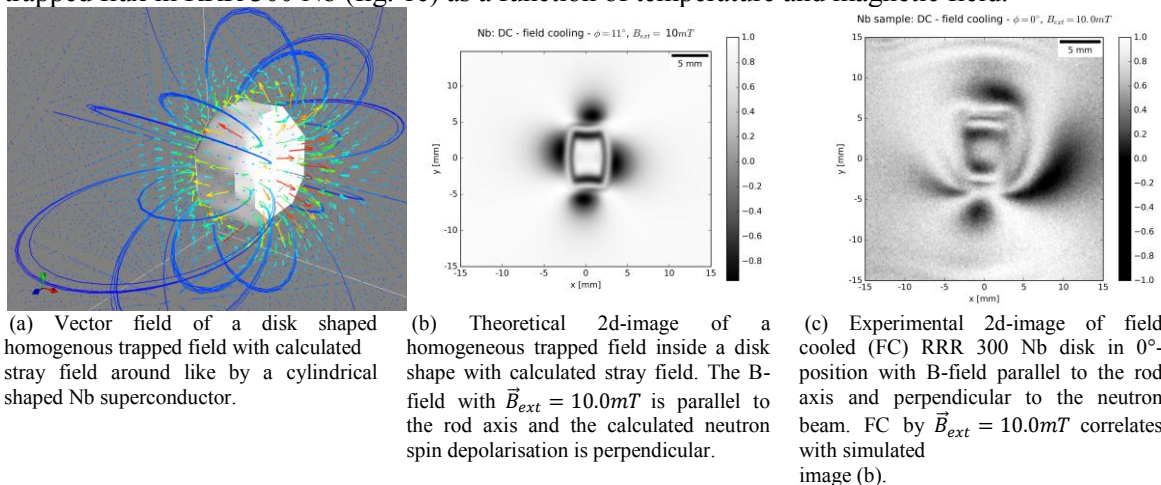


Figure 1: Images of the simulated magnetic stray field (a), the simulated polarised neutron image (b) with $\vec{B}_{ext} = 10.0mT$ which correlates with the experimental obtained image (c) with $\vec{B}_{ext} = 10.0mT$

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List of participants

List of Participants

Edward ANDO

CNRS - INPG - UJF
Laboratoire 3S
Université Joseph Fourier
BP 53 X
FR - 38041 GRENOBLE Cedex
FRANCE

Email: edward.ando@3sr-grenoble.fr

Jose BARUCHEL

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: baruchel@esrf.fr

Georges-Pierre BONNEAU

CNRS UMR 5224
Laboratoire Jean Kuntzmann
Tour IRMA
51 rue des Mathématiques
B.P. 53
FR - 38041 GRENOBLE 9
FRANCE

Email: Georges-Pierre.Bonneau@inria.fr

Elena BORISOVA

Paul Scherrer Institute
Swiss Light Source/TOMCAT
CH - 5232 VILLIGEN
SWITZERLAND

Email: lenabori@gmail.com

Stefan BRANDSTETTER

Dectris Ltd.
Neuenhoferstr. 107
CH - 5400 BADEN
SWITZERLAND

Email: stefan.brandstetter@dectris.com

Luca BROMBAL

University of Trieste
Laboratori INFN
Aera di Ricerca
Padriciano 99
IT - 34100 TRIESTE
ITALY

Email: luca.brombal@ts.infn.it

Emmanuel BRUN

INSERM U836 - ESRF
ID17 Medical Beamline - Equipe 6
Grenoble - Institute of Neuroscience
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: emmanuel.brun@esrf.fr

Peter CLOETENS

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: cloetens@esrf.fr

Alessandro COLOMBO

Universita di Milano
Dipartimento di Fisica
Via Celoria 16
IT - 20133 MILANO
ITALY

Email: alessandro.colombo6@unimi.it

Marine COTTE

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: cotte@esrf.fr

Francois CURNIER

Digisens
3D CT
19 Rue Lac Saint André
Bat Le Fennec
FR - 73 370 BOURGET-DU-LAC
FRANCE

Email: francois.curnier@digisens.fr

Wout DE NOLF

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: wout.de_nolf@esrf.fr

Ella DE PAUW

Ghent University
Department of Analytical Chemistry
Krijgslaan 281 - S12
BE - 9000 GHENT
BELGIUM

Email: ella.depauw@hotmail.com

Aurelie DEHLINGER

Technische Universität Berlin
Institut fuer Optik und Atomare Physik (IOAP)
ER1-1
Hardenbergstrasse 36A
DE - 10623 BERLIN
GERMANY

Email: aurehlinger@hotmail.de

Sandro DONATO

Universita di Trieste
Dipartimento di Fisica
Via A Valerio 2
IT - 34127 TRIESTE
ITALY

Email: sandro.donato@fis.unical.it

Stefan EISEBITT

Max-Born-Institut
B
Max-Born-Str. 2a
DE - 12489 BERLIN-ADLERSHOF
GERMANY

Email: eisebitt@mbi-berlin.de

Vincent FAVRE-NICOLIN

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: favre@esrf.fr

Barbara FAYARD

NOVITOM
SAS
1, place Firmin Gautier
FR - 38000 GRENOBLE
FRANCE

Email: barbara.fayard@novitom.com

Claudio FERRERO

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: ferrero@esrf.fr

Gaetan GIRARD

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: gaetan.girard@esrf.fr

Manuel GUIZAR SICAIROS

Paul Scherrer Institut
CH - 5232 VILLIGEN
SWITZERLAND

Email: manuel.guizar-sicairos@psi.ch

Stanislav HRIVŇAK

Pavol Jozef Safarik University in Kosice
Institute of Physics
Faculty of Science
Park Angelinum 9
SK - 040 01 KOSICE
SLOVAKIA

Email: stano.hrivnak@gmail.com

Paul Hans KAMM

Helmholtz Zentrum Berlin
Institute of Applied Materials (IAM/F-11)
Hahn-Meitner-Platz 1
DE - 14109 BERLIN
GERMANY

Email: paul.kamm@helmholtz-berlin.de

Neelima KANDULA

University of Oslo
Physics of Geological Processes
Sem Selands Vei 24
P O Box 1048 Blindern
NO - 0316 OSLO
NORWAY

Email: 91neelimak@gmail.com

Birgit KANNGIESSER

Technical University of Berlin
Institute for Optics and Atomic Physics
Hardenbergstrasse 36
DE - 10623 BERLIN
GERMANY

Email: Birgit.Kanngiesser@tu-berlin.de

Andrew KING

Synchrotron Soleil
L Orme des Merisiers
Saint-Aubin
BP 48
FR - 91192 GIF-SUR-YVETTE Cedex
FRANCE

Email: andrew.king@synchrotron-soleil.fr

Max LANGER

CNRS UMR 5515 - INSA 502
CREATIS
Bât Blaise Pascal
7 av. Jean Capelle
FR - 69621 VILLEURBANNE
FRANCE

Email: max.langer@esrf.fr

Gabriele Natale LANZAFAME

Sincrotrone Trieste
Synchrotron Radiation for Medical Physics
SS 14 Km 163- 5
Area Science
Basovizza
IT - 34012 TRIESTE
ITALY

Email: gabriele.lanzafame@elettra.eu

Eberhard LEHMANN

Paul Scherrer Institute
Laboratory for Neutron Scattering
PSI Villigen
CH - 5232 VILLIGEN
SWITZERLAND

Email: eberhard.lehmann@psi.ch

Bi-Hsuan LIN

National Synchrotron Radiation Research Ctr
Hsinchu Science Park
101 Hsin-Ann Rd
TW - 30076 HSINCHU
TAIWAN

Email: bihsuan@nsrrc.org.tw

Wolfgang LUDWIG

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: ludwig@esrf.fr

Viviane LUTZ BUENO

Paul Scherrer Institut
Coherent X-Ray Scattering Group (cSAXS) / SLS
PSI West
CH - 5232 VILLIGEN
SWITZERLAND

Email: viviane.lutz-bueno@psi.ch

Lara MALDANIS CERQUEIRA PERES

Brazilian Synchrotron Light National Lab-LNLS
Research Centre Energy & Materials (CNPEM)
P.O. Box 6192
BR - 13083970 CAMPINAS
BRASIL

Email: lara.maldanis@lnls.br

Federica MARONE WELFORD

Paul Scherrer Institute
Swiss Light Source
PSI Villigen
CH - 5232 VILLIGEN
SWITZERLAND

Email: federica.marone@psi.ch

Dorota MATRAS

Materials Science Centre
School of Materials
Grosvenor Street
GB - M13 9PL MANCHESTER
UK

Email: matras.dorota@gmail.com

Ali MOHAMMAD-DJAFARI

CNRS
L2S Laboratoire des Signaux et Systèmes
CentraleSupélec, 3 rue Joliot Curie
FR - 91192 GIF-SUR-YVETTE
FRANCE

Email: djafari@lss.supelec.fr

Rajmund MOKSO

Lund University
MAX IV Laboratory
Fotogatan 2
SE - 22592 LUND
SWEDEN

Email: rajmund.mokso@maxiv.lu.se

Markus OSTERHOFF

Georg-August University of Göttingen
Institut für Roentgenphysik
Friedrich-Hund-Platz 1
DE - 37077 GÖTTINGEN
GERMANY

Email: mosterh1@gwdg.de

Serena PACILE'

Elettra - Sincrotrone Trieste
SS 14 Km 163- 5
Area Science Park
Basovizza
IT - 34012 TRIESTE
ITALY

Email: serena.pacile@elettra.eu

Judith PETERS

Institut Laue-Langevin - ILL
71 avenue des Martyrs
CS 20156
FR - 38042 GRENOBLE Cedex 9
FRANCE

Email: peters@ill.fr

Sophie REDFORD

Paul Scherrer Institut
CH - 5232 VILLIGEN
SWITZERLAND

Email: sophie.redford@psi.ch

Claudine ROMERO

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: claudine.romero@esrf.fr

V. Armando SOLÉ

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: sole@esrf.fr

Jakob SOLTAU

Georg-August University of Göttingen
Institut für Roentgenphysik
Friedrich-Hund-Platz 1
DE - 37077 GÖTTINGEN
GERMANY

Email: jakob.soltau@stud.uni-goettingen.de

Paul TAFFOREAU

ESRF
71 avenue des Martyrs
CS 40220
FR - 38043 GRENOBLE Cedex 9
FRANCE

Email: paul.tafforeau@esrf.fr

Alessandro TENGATTINI

CNRS UMR 5521
Laboratoire 3SR
Domaine universitaire
BP53
FR - 38041 GRENOBLE Cedex 09
FRANCE

Email: alessandro.tengattini@gmail.com

Tobias THIEDE

Bundesanstalt für Materialforschung
Unter den Eichen 87
DE - 12205 BERLIN
GERMANY

Email: tobias.thiede@bam.de

Antonios VAMVAKEROS

University College London
Department of Chemistry
20 Gordon Street
GB - WC1H OAJ LONDON
UK

Email: antonios.vamvakeros.12@ucl.ac.uk

Jerome VICENTE

IUSTI - Polytech Marseille
Technopole de Chateau-Gombert
5 rue Enrico Fermi
FR - 13453 MARSEILLE
FRANCE

Email: jerome.vicente@univ-amu.fr

Gioacchino VIGGIANI

CNRS UMR 5521
Laboratoire 3SR
Domaine universitaire
BP53
FR - 38041 GRENOBLE Cedex 09
FRANCE

Email: cino.viggiani@3sr-grenoble.fr

Nina Kølln WITTIG

Aarhus University
Interdisciplinary Nanoscience Center
Gustav Wieds Vej 14
Aarhus C
DK - 8000 AARHUS
DENMARK

Email: nkw@chem.au.dk

Simon ZABLER

Fraunhofer IIS
Fraunhofer EZRT
Campus Hubland Nord
Josef-Martin-Weg 63
DE - 97074 WÜRZBURG
GERMANY

Email: simon.zabler@iis.fraunhofer.de

Marie-Christine ZDORA

University College London
Department of Physics & Astronomy
Gower Street
GB - WC1E 6BT LONDON
UK

Email: marie-christine.zdora@diamond.ac.uk

Yi ZHENG

Technical University of Denmark
Department of Physics
DTU Physics
Building 307
DK - 2800 LYNGBY
DENMARK

Email: yizhe@fysik.dtu.dk

Ralf ZIESCHE

University College London
Chemical Engineering
Torrington Place
GB - WC1E 7JE LONDON
UK

Email: ralf.ziesche.16@ucl.ac.uk