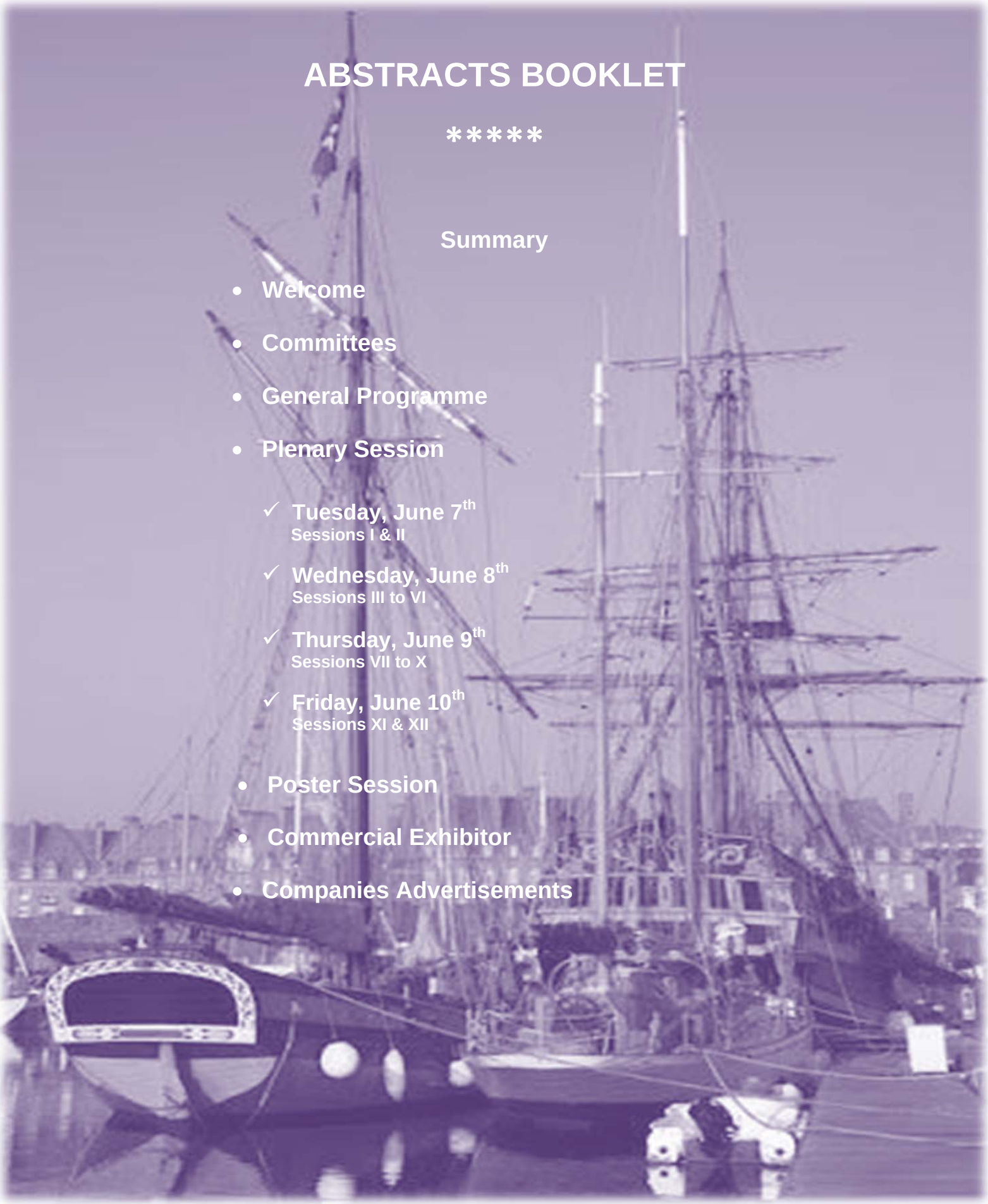
COHERENCE 2016

International Workshop on Phase Retrieval and Coherent Scattering

LE GRAND LARGE – SAINT MALO

7th – 10th JUNE 2016



ABSTRACTS BOOKLET

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Summary

International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Palais des Congrès Le Grand Large - Saint-Malo, France

June 7th - June 10th, 2016

Conference organization:

Partnerships:

Sponsors:

Welcome

The International Workshop on Phase Retrieval and Coherent Scattering, now a biennal conference, first took place at Lawrence Berkeley Lab. in May 2001 and is traditionally held in a waterside location (Palm Cove, Porquerolles, Asilomar, Warnemüde Fukuoka, and Evanston). The 2016 edition is held in France, in the conference center “Le Grand Large”, in front of the sea, in the corsair city of Saint Malo, top tourist and historic spot of Brittany located 400 km from Paris and 60 km from the famous Mont Saint Michel.

A team of French researchers has gathered around synchrotron-SOLEIL to organize this 2016 edition. As for the previous editions, the topics addressed is coherent imaging, structure and dynamics, theorical and computational methods and progress in new X or XUV sources, from high brilliance synchrotron to X-ray free electron lasers.

Bienvenue

La Rencontre internationale sur la restitution de phase et la diffusion cohérente (International Workshop on Phase Retrieval and Coherent Scattering), maintenant biennale, dont la première édition s’est tenue à Lawrence Berkeley Lab. en mai 2001, se déroule traditionnellement dans une cité maritime (Palm Cove, Porquerolles, Asilomar, Warnemünde, Fukuoka et Evanston). L’édition de 2016 a lieu en France dans la cité corsaire de Saint Malo, haut lieu historique et touristique de Bretagne, situé à 400 km de Paris et à 60 km du Mont Saint Michel. Le lieu de la conférence se situe, en face de la mer, au Grand Large, le palais des congrès de Saint Malo.

Une équipe de chercheurs représentant la communauté française de cohérence s’est regroupée autour du synchrotron SOLEIL pour organiser cette édition 2016. Comme pour les dernières Rencontres, les thèmes abordés sont l’imagerie cohérente, la dynamique, les méthodes d’analyse et la théorie, ainsi que l’apport des nouvelles sources X ou XUV, synchrotrons de haute brillance ou lasers à électrons libre.

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International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Palais des Congrès Le Grand Large - Saint-Malo, France

June 7th - June 10th, 2016

Programme

Tuesday, June 7th

13:00 - 14:30 Registration
14:30 - 15:00 Welcome & opening introduction by V. Chamard & S. Ravy

Session I – XPCS
Chairperson: V. Chamard

15:00 - 15:40 The MID station at the European XFEL: Plans for coherent scattering and imaging using XFEL radiation
A. Madsen *- European XFEL, Hamburg, Germany*

15:40 - 16:00 Simulations of coherent X-ray scattering from dynamic crystal surfaces
G. Brian Stephenson *- Argonne National Laboratory, Argonne, IL, USA*

16:00 - 16:20 An XPCS study of driven domain dynamics in a ferroelectric single crystal
Mario Reiser *- Universität Siegen, Germany*

16:20 - 16:50 Coffee break

Session II - CDI-FEL
Chairperson: G. Beutier

16:50 - 17:30 Studies of nanoscale dynamics and in-situ strain development using coherent X-rays
Hyunjung Kim *- Sogang University, Seoul, Korea*

17:30 - 17:50 Quantitative single-shot 3D imaging of core-shell nanocrystals with elemental specificity
Alan Pryor Jr *- University of California Los Angeles, USA*

17:50 - 18:10 3D merging: Getting more from protein crystallography
Oleksandr M. Yefanov *- DESY, Hamburg, Germany*

19:30 Welcome Cocktail

Wednesday, June 8th

Session III - CDI
Chairperson: S. Labat

08:30 - 09:10 Single particle imaging at the linac coherent light source
Andrew Aquila *- SLAC National Accelerator Laboratory, Menlo Park, CA, USA*

09:10 - 09:30 Resolution extension of imperfect crystal diffraction using iterative phasing
Kartik Ayyer *– DESY, Hamburg, Germany*

09:30 - 09:50 Multiple defocused CXDI: A method for simultaneous reconstruction of isolated samples and probe using XFELs
Makoto Hirose *- Osaka University and RIKEN SPring-8 Center, Hyogo, Japan*

09:50 - 10:10 Coherent X-ray imaging of semi-conductor nano-structures for photonic and electronic applications
Vincent Favre-Nicolin *- ESRF and Université Grenoble Alpes, France*

10:10 - 10:30 Multiprojection setup for single-shot imaging
Pablo Villanueva-Perez *- Paul Scherrer Institut, Villigen, Switzerland*

10:30 - 11:00 Coffee break

Session IV – Other sources
Chairperson: D. Le Bolloc'h

11:00 - 11:40 Spectrally resolved imaging with ultra-broadband high-harmonic generation sources
Stefan Witte *- Advanced Research Center for Nanolithography, Amsterdam and LaserLaB, Amsterdam, The Netherlands*

11:40 - 12:00 3D stereo single acquisition imaging using high harmonic generation
Remy Cassin *- LIDyL, Gif-sur-Yvette, France*

12:00 - 12:40 Progress in electron ptychography
Andrew M. Maiden *- University of Sheffield, UK*

12:40 - 13:30 Lunch

Session V – Ptychography
Chairperson: S. Ravy

13:30 - 14:10 Utilizing Fourier projections to enable flexible three dimensional Bragg CDI and Bragg ptychography approaches
Stephan.O. Hruszkewycz *- Argonne National Laboratory, Argonne, IL, USA*

14:10 - 14:30 Soft X-ray coherent scattering and ptychography using BK focusing optics
Di-Jing Huang *- National Synchrotron Radiation Research Center, Hsinchu, Taiwan*

14:30 - 14:50 Ptychography in terms of an expansion in elementary signals
Julio Cesar da Silva *– ESRF, Grenoble, France and Paul Scherrer Institut, Villigen, Switzerland*

14:50 - 15:00 Break

Session VI – CDI
Chairperson: M-I. Richard

15:00 - 15:40 Using coherent X-rays to understand the physics of correlated electrons systems
Vincent Jacques - *Laboratoire de Physique des Solides, Orsay, France*

15:40 - 16:00 X-ray phase-contrast imaging using near-field speckle techniques
Marie-Christine Zdora *- Diamond Light Source, Didcot and University College London, UK*

16:00 - 16:20 Coherent diffractive imaging of thin film bulk heterojunctions for polymer solar cells
Nilesh Patil *– Norwegian University of Science and Technology, Trondheim, Norway*

16:20 - 16:50 *Coffee break*

16:50 - 19:30 Poster Session I

Thursday, June 9th

Session VII - XPCS
Chairperson: M. Sutton

08:30 - 09:10 Dynamics of a colloidal glass
Barbara Ruzicka *- ISC-CNR, Sapienza Università, Roma, Italy*

09:10 - 09:30 Anisotropic De Gennes narrowing in confined fluids
Yuriy Chushkin *– ESRF, Grenoble, France*

09:30 - 09:50 Structure beyond pair correlations: Higher-order correlation functions for soft matter systems
Felix Lehmkühler *– DESY, Hamburg, Germany*

09:50 - 10:10 Structural origin of the anomalous dynamics of metallic glasses
Beatrice Ruta *– ESRF, Grenoble, France*

10:10 - 10:30 New pixel array detector techniques for X-ray photon correlation spectroscopy experiments
Eric Dufresne *- Argonne National Laboratory, Lemont, IL, USA*

10:30 - 11:00 Coffee break

Session VIII - Holographic methods
Chairperson: N. Jaouen

11:00 - 11:40 Time-resolved holographic X-ray imaging of magnetic nanostructures
Bastian Pfau *- Max-Born-Institut, Berlin, Germany*

11:40 - 12:00 Probing magnetization dynamics by time-resolved X-ray holography with extended references
Feodor Ogrin *– University of Exeter, UK*

12:00 - 12:20 X-ray holographic imaging of magnetic domains at the Sextants beamline of the Soleil Synchrotron
Horia Popescu *– Synchrotron Soleil, Gif-sur-Yvette, France*

12:20 - 13:30 Lunch

Session IX - Methods
Chairperson: I. Vartaniants

13:30 - 14:10 High throughput nanoscale coherent x-ray imaging
Stefano Marchesini *- Lawrence Berkeley National Laboratory, Berkeley, CA USA*

14:10 - 14:30 Near field probe retrieval and imaging at partial coherence conditions
Johannes Hagemann *- Georg August University Göttingen, Germany*

14:30 - 14:50 Phase of the transmitted wave in the dynamical theory and quasi-kinematical approximation
Oleg Gorobtsov *- DESY, Hamburg, Germany and Akademika Kurchatova, Moscow, Russia*

14:50 - 15:00 Break

Session X - CDI
Chairperson: H. Kim

15:00 - 15:40 Structural X-ray studies of nanostructures using Bragg CDI at the ID01 beamline
Marie-Ingrid Richard *– Aix-Marseille Université and ESRF, Grenoble, France*

15:40 - 16:00 Imaging of the quantum well in core-shell-shell nanowires
Arman Davtyan *- University of Siegen, Germany*

16:00 - 16:20 Quantitative interior ptychographic nanotomography
Manuel Guizar Sicairos *- Paul Scherrer Institut, Villigen, Switzerland*

16:20 - 16:50 Coffee break

16:50 - 19:00 Poster Session II

20:00 Conference Dinner at Saint-Malo

Friday, June 10th

Session XI - CDI
Chairperson: O. Thomas

08:30 - 09:10 Frontiers of X-ray science developed with coherent X-rays of SACLA
Makina Yabashi *- RIKEN SPring-8 Center, Hyogo, Japan*

09:10 - 09:30 Massive faulting of gold nanocrystals upon alloying with iron
Ana Katrina Estandarte *- University College London, and Research Complex at Harwell, Didcot, UK*

09:30 - 09:50 On the origin of biomimetic $CaCO_3$ complex morphologies
Thomas Beuvier *- ESRF, Grenoble, France*

09 :50 - 10:10 X-ray coherent diffractive imaging of defects in bio-photonic crystals inside butterfly wing scales
Andrej Singer *– University of California-San Diego, La Jolla, USA*

10:10 - 10:30 Coherent Bragg imaging of crystal defects during in situ indentation
Maxime Dupraz *– SIMaP, Grenoble, France and Paul Scherrer Institut, Villigen, Switzerland*

10:30 - 11:00 Coffee break

Session XII - Ptychography
Chairperson: F. Berenguer

11:00 - 11:40 Applications of X-ray ptychography at the Swiss Light Source
Ana Diaz *- Paul Scherrer Institut, Villigen, Switzerland*

11:40 - 12:00 X-ray ptychography: Fast, cold, colorful, and sharp
Chris Jacobsen *- Northwestern University, Evanston IL and Argonne National Laboratory, Argonne IL, USA*

12:00 - 12:20 Dark-field X-ray ptychography: High-resolution imaging of weak-phase objects
Nicolas Burdet *- RIKEN SPring-8 Center, Hyogo, Japan*

12:20 - 12:30 Conclusion

PLENARY SESSION

Tuesday, June 7th, 2016

SESSIONS I & II

International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Tuesday, June 7th, 2016

SESSION I
XPCS

Chairperson: V. CHAMARD

IT-01 The MID station at the European XFEL: Plans for coherent scattering and imaging using XFEL radiation
A. Madsen

OC-01 Simulations of coherent X-ray scattering from dynamic crystal surfaces
G.B. Stephenson

OC-02 An XPCS study of driven domain dynamics in a ferroelectric single crystal
M. Reiser

SESSION II
CDI-FEL

Chairperson: G. BEUTIER

IT-02 Studies of nanoscale dynamics and in-situ strain development using coherent X-rays
H. Kim

OC-03 Quantitative single-shot 3D imaging of core-shell nanocrystals with elemental specificity
A. Pryor Jr

OC-04 3D merging: Getting more from protein crystallography
O.M. Yefanov

The MID Station at the European XFEL: Plans for Coherent Scattering and Imaging using XFEL Radiation

A. Madsen

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ABSTRACT

A detailed description of the future Materials Imaging and Dynamics (MID) station [1] at the European XFEL is given with emphasis on the science it enables. In particular scattering and imaging experiments exploiting the coherence and pulsed nature of the radiation are of interest but many of the experimental schemes developed for synchrotron sources, e.g. concerning CDI and XPCS, will need adaptation. Preliminary work towards these novel schemes has begun with some success. The MID station is expected to receive first light in 2017 and begin regular user operation in 2018.

REFERENCES

1. Technical Design Report: Scientific Instrument MID, doi:10.3204/XFEL.EU/TR-2013-005
https://bib-pubdb1.desy.de/record/154260

Simulations of Coherent X-ray Scattering from Dynamic Crystal Surfaces

G.B. Stephenson[1], D. Xu[1], G. Ju[1], A. Ulvestad[1], C. Thompson[2], P. Zapol[1], M.J. Highland[1], and P.H. Fuoss[1]

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[2]*Department of Physics, Northern Illinois University, DeKalb, IL, USA*

ABSTRACT

In-situ scattering with penetrating hard x-rays provides direct insight into the atomic scale mechanisms of materials synthesis.[1] With the expected continued increase in coherent flux at high x-ray energies delivered by advanced synchrotron radiation facilities, x-ray photon correlation spectroscopy and related techniques promise to become powerful tools for *in-situ* studies of synthesis, revealing the atomic-scale fluctuation dynamics[2] that underlies technologically important processes such as epitaxial crystal growth.

Here we present simulations of speckle dynamics in coherent scattering from crystal surfaces, both at equilibrium in the growth environment at high temperature, and during non-equilibrium crystal growth. For equilibrium crystal surfaces, standard single-q time correlation functions reveal the dynamics of defects such as steps and adatoms. For non-equilibrium surfaces undergoing growth, we calculate two-time and other higher-order correlation functions, and investigate how they can elucidate aspects of island nucleation, step-edge barriers, and transport mechanisms more clearly than average quantities obtained from scattering with incoherent beams. Initial exploration of surface coherent diffraction imaging will also be discussed.

Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering.

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An XPCS Study of Driven Domain Dynamics in a Ferroelectric Single Crystal

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ABSTRACT

We measured the electric field driven domain dynamics of a $Sr_xBa_{1-x}Nb_2O_6$ (SBN) single crystal[1] by means of x-ray photon correlation spectroscopy (XPCS) of the diffuse scattering in the vicinity of the [001] Bragg peak.

Below the *Curie-temperature* the physical properties of ferroelectric materials strongly depend on the behavior of ferroelectric domains of different polarization. The emergence of domains and in particular their change under external and internal fields has been part of scientific investigations for many years[1]-[9].

Of particular interest is the relation between domain walls and disorder in the form of pinning centers[6], which mainly determines the energy landscape and, therefore, the domain structure of the crystal. Thus, the understanding of their correlation accompanied by the possibility of manipulating the behavior of domains is crucial for the application of ferroelectrics, e.g., in data storage devices[4],[5].

We used a detailed cross-correlation based analysis of speckle patterns allowing the simultaneous mapping of the energy landscape and the corresponding domain pattern on atomic length scales. The correlation functions show a periodical partial recovery of the domain pattern. From the analysis we deduce the degree of domain pattern recovery and the critical external electric field needed for domain switching when cycling though the hysteresis loop. The observed fluctuations in terms of domain switching give a direct insight into the complex energy landscape of domain wall motion in ferroelectric materials.

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Studies of Nanoscale Dynamics and In-situ Strain Development using Coherent X-rays

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ABSTRACT

The recent advent of hard x-ray free electron lasers (XFELs) opens new areas of science due to their exceptional brightness, coherence, and time structure. In principle, such sources enable studies of dynamics of condensed matter systems over times ranging from femtoseconds to seconds. However, the studies of the dynamics in, for example, polymeric materials still remain in question due to the characteristics of the XFEL beam and concerns about sample damage.

In the first part of my talk, I present the results obtained in LCLS on the relaxation dynamics of gold nanoparticles suspended in polymer melts using X-ray photon correlation spectroscopy (XPCS), while monitoring eventual X-ray induced damage. In spite of inherently large pulse-to-pulse intensity and position variations of the XFEL beam, measurements can be realized at slow time scales. The X-ray induced damage and heating are less than initially expected for soft matter materials. In the second, I show the recent results of in situ internal strain development of zeolites along the catalysis by coherent X-ray diffraction imaging in LCLS.

This research was supported by the National Research Foundation of Korea (Nos. NRF-2014R1A2A1A10052454, 2015R1A5A1009962, 2016R1A6B2A02005468) and Samsung Electronics and Samsung Display.

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Quantitative Single-shot 3D Imaging of Core-shell Nanocrystals with Elemental Specificity

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ABSTRACT

Core-shell nanocrystals exhibit unique electronic, chemical and optical properties that have found broad applications across several disciplines. Conventional methods to characterize these nanocrystals are based on transmission electron microscopy, scanning probe microscopy, X-ray diffraction and scattering techniques. Here we report quantitative single-shot 3D imaging of core-shell nanocrystals with elemental specificity through the combination of coherent diffractive imaging (CDI) and an X-ray free electron laser (XFEL). While single pulses from XFELs provide high-resolution signal from nanostructed objects, the pulses are inherently destructive. Therefore, obtaining 3D information from a single pulse is an important challenge. We demonstrate the applicability of single-shot imaging using an XFEL for nanoscale objects by recovering the 3D structure of a core-shell nanocube with a 65.0 ± 1.0 nm gold core and a 4.0 ± 0.5 nm thick palladium shell. We establish an automated and quantitative routine for analyzing nanostructures, which we apply to 34 isolated cubes. We use the curvature of the diffraction patterns and symmetry intrinsic to the nanocubes as constraints during the reconstruction process to recover highly reproducible quantitative 3D structures from single patterns with a 3D resolution of ~5nm on ~10 femtosecond timescales. The recovered nanocubes match the expected scattering ratio for their two elemental components (Au/Pt ratio) to within a 2% deviation from theoretical values. This level of accuracy lends itself to quantitative high-resolution analysis of symmetric nanostructures in high-throughput fashion.

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3D Merging: Getting More from Protein Crystallography

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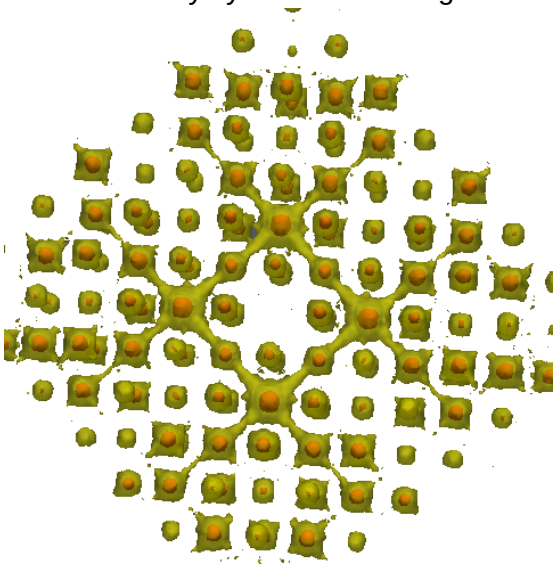
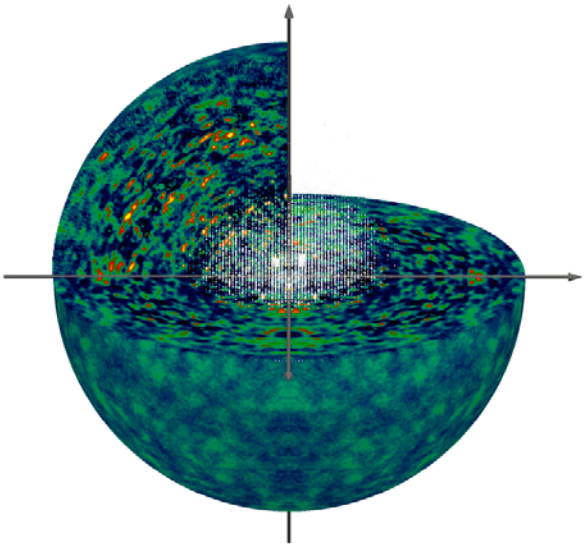
ABSTRACT

For decades protein crystallography was one of the best methods for biological structure determination. Its popularity is governed by the fact that highly ordered structures produce intensive Bragg peaks which are easy to detect and measure. At the same time the scattering between Bragg peaks is usually very weak, therefore it was usually neglected. Modern sources, like Free Electron Lasers (FELs) and 3rd generation synchrotrons combined with the new techniques such as Serial Femtosecond Crystallography (SFX) allow to increase the dynamical range of measured signal and therefore measure scattering between Bragg peaks.

In SFX at FELs individual crystals are introduced one after another into the X-ray beam and exposed to a single X-ray pulse. In this way thousands of measurements of crystal in random orientations are measured. All those measurements are merged in three dimensions. This method reveals the underlying continuous three-dimensional reciprocal space intensity distribution. For example Bragg peaks asymmetry and intensities between Bragg peaks (left figure) [1] as well as continuous diffraction at resolution beyond Bragg peaks (right figure) [2]. The analysis of such 3D intensity distribution can reveal additional structure information, improve resolution, and can potentially be used for ab initio structure reconstruction.

One of the issues for success of such experiments is removing background from solution which is usually much higher than the useful signal. Therefore we've developed a method to remove radially symmetrical background based on Willson statistics [3].





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PLENARY SESSION

Wednesday, June 8th, 2016

SESSIONS III, IV, V & VI

International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Wednesday, June 8th, 2016

SESSION III
CDI

Chairperson: S. LABAT

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Single Particle Imaging at the Linac Coherent Light Source

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ABSTRACT

The Single Particle Imaging (SPI) Initiative is a community-involved initiative tasked with the goal of overcoming the technical challenges for reaching better and ultimately atomic resolution in X-ray imaging of single-particles. It has more than 100 participating members from 21 institutions spanning 8 countries. Since its inception, one year ago, the SPI Initiative has completed seven experiment at the Linac Coherent Light Source (LCLS) using two different beamtimes; this talk will review the results/technical discoveries from each of the SPI beamtimes and discuss how the field has progressed.

Resolution Extension of Imperfect Crystal Diffraction using Iterative Phasing

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ABSTRACT

Most protein crystals are not very closely packed. This results in translational and some rotational disorder from molecule to molecule in some crystals. When exposed to X-rays, in addition to the falloff of Bragg peak intensities with q, one obtains continuous diffraction which is closely related to the diffraction from a single protein making up that crystal. In crystallography, this high-resolution speckle data is not used for structure determination, since there are no Bragg peaks. However, iterative phasing algorithms can be used to phase this high-resolution continuous diffraction.

We discuss a method to use this data and phase the intensities to get a higher resolution structure than can be obtained from just the Bragg peaks. In addition to the theory, we will show an application with real data from photosystem-II microcrystals measured at the LCLS free-electron laser. We will also discuss the applicability of this method for other proteins and at synchrotron source.

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Multiple Defocused CXDI: A Method for Simultaneous Reconstruction of Isolated Samples and Probe using XFELs

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ABSTRACT

The sample size must be less than diffraction-limited focal spot size, which is currently a major limitation for wider applications of single-shot CXDI based on a diffraction-before-destruction scheme using X-ray free electron lasers (XFELs). To overcome this limitation, we here propose multiple Fresnel CXDI. Fresnel CXDI is a CXDI method involving curved beam illumination [1]. Multiple Fresnel CXDI can simultaneously reconstruct both the probe and isolated objects that are larger than the diffraction-limited focal spot size from multiple diffraction patterns alone. In multiple Fresnel CXDI, a focused X-ray is sequentially irradiated to isolated samples in the defocal plane. Multiple diffraction data are collected in the far field. Both the objects and the probe are reconstructed from the diffraction patterns using an improved phase retrieval algorithm with a mixed-state reconstruction algorithm [2]. Here we report the result of a proof-of-principle experiment on multiple Fresnel CXDI performed at SPring-8 BL29XUL.

Thirty-two isolated objects of ~2 μm size were prepared on a SiN membrane as the sample. A monochromatic 6.5 keV X-ray was two-dimensionally focused to a spot size of 500 nm (FWHM). The sample was positioned 10 mm downstream of the focal plane. Thirty-two diffraction patterns were recorded by a CCD detector. Images of both the objects and the probes were successfully reconstructed from the diffraction patterns as shown in Fig. 1. The present method allows us to not only observe broad samples but also characterize focused XFELs.

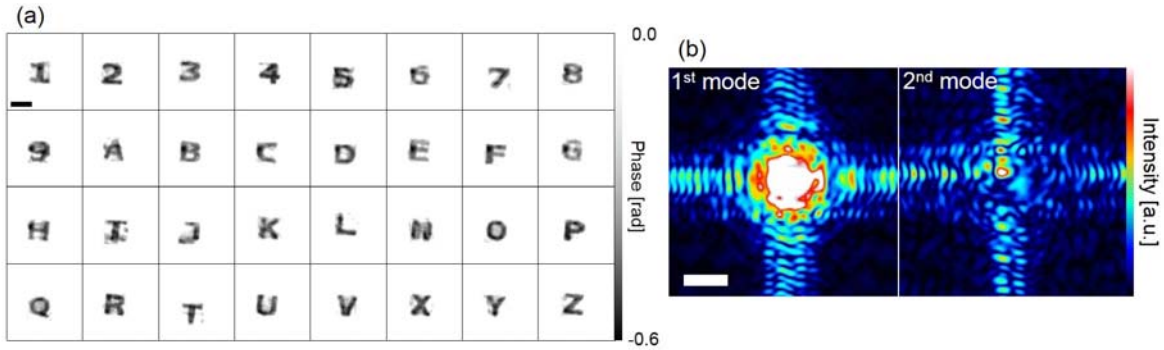

Figure 1 Reconstruction by multiple Fresnel CXDI. (a) Phase images of the thirty-two isolated objects. (b) Wavefront of the two independent probes. The scale bar is 2 □m.

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Coherent X-ray Imaging of Semi-conductor Nano-structures for Photonic and Electronic Applications

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ABSTRACT

The last 20 years have seen a massive development of crystalline structures with sub-micrometer sizes, either with a simple miniaturization goal, or in order to exploit quantum confinement effects. The study of these objects is a challenge for crystallographers, as their size implies a weak, diffuse scattering rather than sharp Bragg peaks. Moreover, nano-structures, either due to the synthesis method or by design, are often heterogeneous and therefore present inhomogeneous strain and com- position 3D fields.

Thanks to the development of focused X-ray optics, it is now possible to measure the scattering from single nano-objects using X-ray Coherent Diffraction Imaging (XCDI) [1,2] and Ptychography. When used in the Bragg geometry, it allows not only recovering the shape (electronic density), but also the deformation field relatively to a perfect lattice, in the case of an inhomogeneous strain.

We will illustrate the use of X-ray nanobeams on single homogeneous and heterogeneous nano- structures [3,4,5] used for photonic (single photon emission) and electronic (strained silicon-on- insulator) applications, and discuss the current performance, limits and prospects of the method, notably to image small structures such as quantum dots. We will also discuss prospects on software development for X-ray coherent diffraction imaging at the ESRF.

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Multiprojection Setup for Single-shot Imaging

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ABSTRACT

The ultrashort and ultraintense pulses provided by X-ray free electron lasers enable to overcome the resolution limitations due to radiation damage for imaging biological materials [1]. Since each pulse destroys the sample, the accessible information in standard imaging approaches is limited to a single projection. We propose an experimental setup for the hard X-ray regime which permits the simultaneous acquisition of multiple projections from the same specimen, similar to that for soft X-rays in Ref. [2]. This technique thus allows acquisition of 3-D information from single-shot measurements, and relies on the simultaneous illumination of the sample with multiple beams generated from the direct beam by a single crystal (see Figure).

We provide an experimental proof-of-principle of this concept at a synchrotron source in both tomographic and coherent diffraction imaging geometries. For the latter, implementation at X-ray free-electron laser is straightforward.

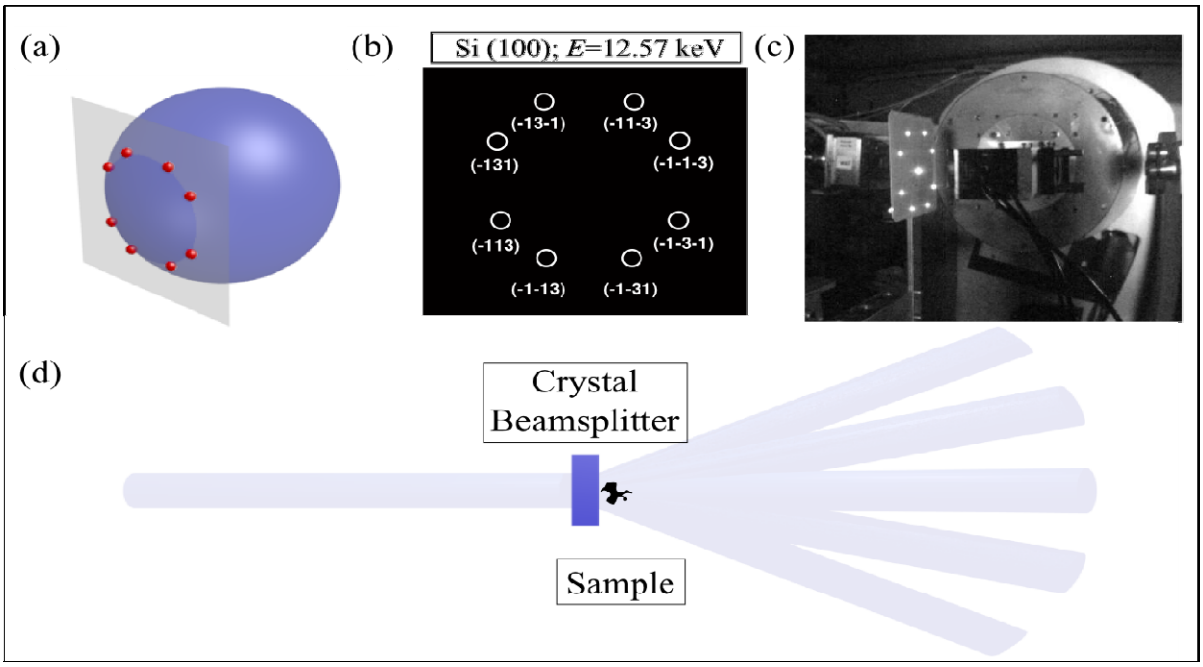

Fig. 1: (a) Ewald sphere intersecting simultaneously a family of equivalent Bragg reflections, related by rotations around a symmetry axis of the silicon crystal. (b) Family of reflections in Bragg condition for silicon at 12.57 keV. (c) Picture of the experimental setup at the MS beamline of the Swiss Light Source, showing the direct beam and the eight diffracted beams on a phosphor screen. (d) Sketch of the concept of the sample being illuminated simultaneously by the direct and diffracted beams.

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Spectrally Resolved Imaging with Ultra-broadband High-harmonic Generation Sources

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ABSTRACT

Microscopy with extreme-ultraviolet (EUV) and soft-X-ray radiation has the potential to provide a unique window into the nanoworld. While the short wavelength radiation enables a resolution on the nanometer scale, inner-shell absorption edges of various elements provide intrinsic contrast and the ability to perform element-selective imaging. As the fabrication of efficient and aberration-free optical components becomes increasingly challenging for such short wavelengths, lensless imaging methods are a powerful alternative for the development of practical high-resolution EUV microscopes.

High-harmonic generation (HHG) sources are promising for imaging applications, as they are compact sources of fully coherent EUV radiation that fit on a laboratory scale optical table. However, HHG sources are intrinsically ultra-broadband, while a major requirement that has remained in diffraction-based imaging is the need for a well characterized spectrally narrowband source. To overcome this limitation and enable efficient imaging with HHG sources, we have developed a new imaging method based on the diffraction of coherent pulse pairs [1].

By recording a series of diffraction patterns as a function of the time delay between two coherent pulses, a Fourier-transform spectrum can be recorded at each pixel in the diffraction pattern. From this dataset, quasi-monochromatic diffraction patterns can be reconstructed throughout the full source spectrum, and the full source flux is used efficiently throughout the entire scan. Combining this two-pulse approach with phase retrieval techniques enables spectrally resolved EUV imaging, or robust image reconstruction through the use of multiple Fresnel diffraction patterns in a multi-wavelength phase retrieval scheme [2]. We have developed a highly stable common-path interferometer to produce the required tunable pulse pairs, which enables application of this two-pulse imaging method even in the soft-X-ray spectral range. I will present the principles and capabilities of our approach, and show recent results on EUV imaging and spectroscopy.

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3D Stereo Single Acquisition Imaging using High Harmonic Generation

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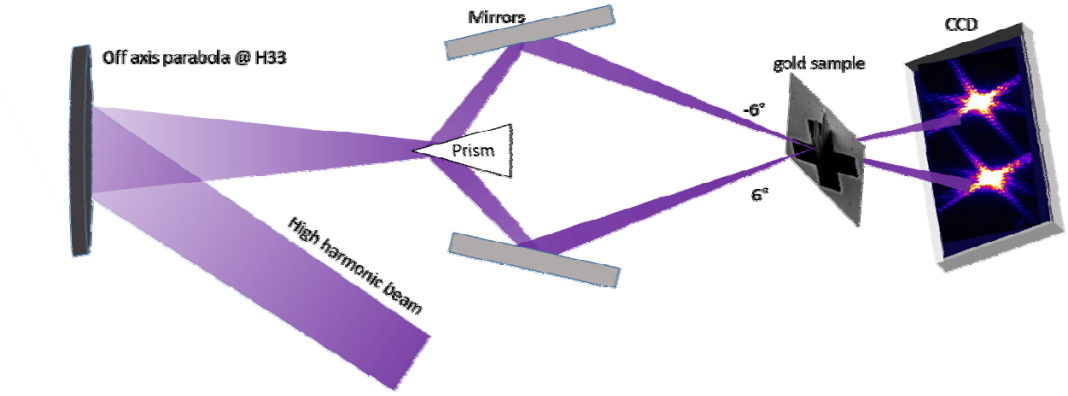
ABSTRACT

In nature, most objects possess complex three dimensional structures. Trying to image them in 2D is often not enough to fully characterize a sample. At a nanometer scale, the ability to gain insights on the 3D properties of artificial or biological thick systems is critical in all fields of science and medicine. The most widely used method for 3D reconstruction of an object is tomography. This method requires at least several hundreds of acquisitions (for each angle) to be able to compute the 3D volume which means that it needs multiple acquisitions. This forbids the study of dynamical processes unless the phenomena is reversible, thus limiting the array of possibilities. Several experiments [1,2,3] using 3D lensless imaging were performed, each time with the same principle: acquiring several sets of 2D transmission images to obtain two views of the sample at a different angles, to finally reconstruct the sample in 3D. Another method to image in 3D is stereo-microscopy [4]: the idea is to acquire two images of an object seen at 2 different angles and combine them in two slices of a color image to see the 3D structure of the object with 3D glasses.



Here we report the first results on a method that enables 3D ultrafast nanoscale imaging in a single acquisition. The experiment was done at the LUCA laser facility at CEA Saclay, France. The goal is to form two monochromatic XUV beams from a high harmonic source and focus them with a known angle on a transmission amplitude sample. The two diffraction patterns are simultaneously recorded on a single CCD camera. We reconstruct the two stereo images thanks to a CDI algorithm. From that pair we can compute the disparity map. Disparity refers to the distance between two corresponding points in the top and bottom images of a stereo pair. The estimated disparity map can be converted into depth information allowing us to partially reconstruct the 3D image of the sample. That method can be applied to thick biological samples using hard-x-rays and to the study of dynamical 3D phenomena in single shot e.g. warm dense matter experiments (dense plasma expansion and collisions).

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Progress in Electron Ptychography

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ABSTRACT

Although ptychography was originally formulated to solve the phase problem in electron microscopy, progress toward a useful, routine method in the electron regime has not matched that of X-ray and visible light counterparts. Hurdles such as inelastic and dynamic scattering, instrument instabilities and limited beam coherence explain the lag. And yet progress *is* being made[1,2], and advances from the X-ray and visible light regions of the spectrum[3,4] are filtering through to the electron world. In this talk I will discuss the trials and tribulations of ptychography on the Transmission Electron Microscope, I will present our latest results and suggest how they can be improved, and I will explain the potential advantages of our approach over through-focus and off-axis holography.

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Utilizing Fourier Projections to Enable Flexible Three Dimensional Bragg CDI and Bragg Ptychography Approaches

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ABSTRACT

In a Bragg coherent x-ray diffraction imaging experiment, the measured two-dimensional diffraction patterns are related to the three-dimensional diffracting crystal via a real space projection and a Fourier transform. Thus, phase retrieval approaches can conceivably be designed that utilize these operations together with their inverse operators: an inverse Fourier transform and a back-projection (often invoked in tomography).

In this talk, we discuss how we applied these concepts to develop new, more flexible phase retrieval strategies for 3D Bragg coherent x-ray diffraction imaging (CDI) experiments. Examples of two new 3D phase retrieval concepts are given that enable new experiments: phasing of single-particle Bragg CDI energy scan measurements, and 3D Bragg projection ptychography from single-angle and sparse-angle data sets. We also discuss opportunities for future science opportunities with such techniques.

Soft X-ray Coherent Scattering and Ptychography using BK Focusing Optics

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ABSTRACT

Soft X-ray spectromicroscopy is a powerful tool which can provide 2D or 3D imaging with chemical, electronic and structural information at the nanoscale. In this presentation, we will present the development of a new soft X-ray spectromicroscope system based on coherent scattering. Using Kirkpatrick-Baez (KB) focusing optics, a soft X-ray elliptically polarizing undulator beamline at the Taiwan Photon Source (TPS) delivers coherent photon flux in the order of 10^{11} $s^{-1}(0.02\%BW)^{-1}$ with a beam size of 3 μm by 3 μm in the energy range from 400 eV to 1200 eV. The spectromicroscope is attached to an in-vacuum diffractometer with two principal rotation axes, 2θ (detector) and θ (sample). The system operates in the transmission or the Bragg refection geometry for ptychography and Bragg coherent diffraction imaging (CDI), respectively. Through the resonance of soft X-ray scattering, a 2D area detector in the reflection geometry is used to image a superstructure diffraction to obtain the spatial information of spin, charge and orbital ordering. For ptychography, the probe is defined by a 0.5-μm pinhole placed 1.5 mm upstream the object and a special platform equipped with sample and pinhole scanning stages is developed.

The presentation will discuss the design and expectation of the instrumentation, test results and the data analysis for imaging strongly correlated electron materials with spectroscopic information at the nanoscale. Future improvements to realize tomographic imaging will also be addressed.

Ptychography in Terms of an Expansion in Elementary Signals

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ABSTRACT

Despite its popularity and the significant progress that allows for reliable practical implementation of ptychography, some of the technique's fundamentals remain poorly understood. Here, we propose a theoretical framework for ptychography [1], which is based on Gabor's notion of decomposition of a signal in elementary signals [2] and the concept of frames [3]. We investigate the redundancy of the ptychographic dataset, which is pivotal for the technique's robustness. The theory yields analytical equations for both the complex transmittance of the sample and the illumination function. Based on the well-established mathematical discipline of windowed Fourier transform, it serves to connect ptychography to well known concepts in signal processing and spectrogram analysis.

In fact, from the representation in the proposed phase-space, linear in both real- and reciprocal-space coordinates (Fig. 1), the sampling requirements of the ptychographic dataset can directly be derived in agreement with previous *ad hoc* approaches [4]. These results are fully compatible with requirements of iterative reconstruction approaches such as the extended ptychographic iterative engine (ePIE) [5] and the difference map [6]. In addition, we could find a criterion for optimizing the scan geometry and the overlap of the illumination. Therefore, our framework enables a better understanding of ptychography and allows the ptychographic sampling and measurement strategies to benefit from well established mathematical theories

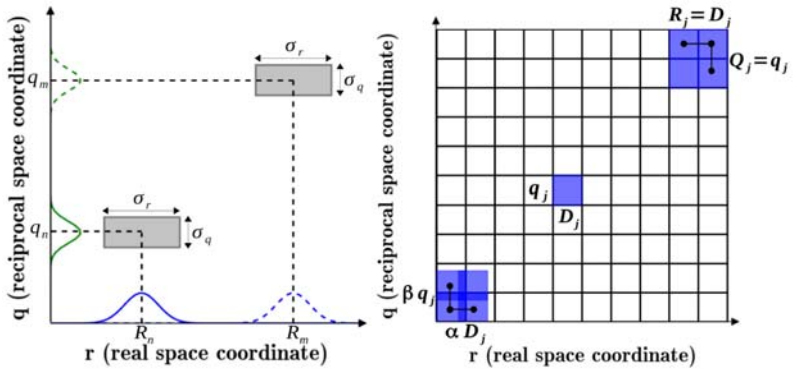

Figure 1: Representation of the ptychography phase-space. (left) The elementary signals as Heisenberg Boxes. (right) Phase-space coverage in critical and oversampling conditions. Figures from ref. [1].

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Using Coherent X-rays to Understand the Physics of Correlated Electrons Systems

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ABSTRACT

Correlated electron systems have a major importance in condensed matter physics, and take diverse and yet intricate forms like superconductivity, Mott insulators, or charge and spin density waves. Depending on the thermodynamical conditions, those phases can appear alone, or coexist.

This talk will focus on spin and charge density wave systems of various dimensionalities. In one dimension, a charge density wave is stabilized if the elastic energy cost due to a periodic lattice distortion (PLD), costs less energy than the electronic energy gain due to the gap opening associated to the PLD [1]. The charge modulation $\rho(\mathbf{r})$ can be written as follows:

$$\rho(\boldsymbol{r}) = \rho_0 + \rho_1 \cos(\boldsymbol{q}_{CDW}.\boldsymbol{r} + \varphi(\boldsymbol{r}))$$

The appropriate quantity to describe those electronic and magnetic periodic modulations is thus the spatially-dependent phase $(\boldsymbol{r})$. The periodic modulation is clearly detectable using x-ray diffraction, as satellite peaks around lattice Bragg reflections. But with conventional x-rays, the phase information is averaged, and all the local variations are lost. Therefore, the use of coherent x-rays is mandatory to probe the local behavior of $(\boldsymbol{r})$. The space-dependent phase has a great importance as it describes pinning of CDW on local defects, which affects the dynamical properties of the CDW submitted to an external force. Moreover, intrinsic phase defects can also appear, like dislocations, either in the static or dynamic regime of CDW, and can only be detected thanks to coherent x-rays.

We will report on results obtained using coherent x-ray diffraction on quasi-1D [2,3] and quasi-2D CDW systems [4], in the static and dynamic regimes, and finally on pure chromium, a 3D system in which spin and charge density waves coexist [5,6].

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X-ray Phase-contrast Imaging using Near-field Speckle Techniques

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ABSTRACT

Methods based on X-ray near-field speckle have recently attracted increased interest in the fields of phase-contrast imaging [1-2] and metrology [3]. Near-field speckles are created by the interference of partially coherent X-rays scattered from a random phase modulator, e.g. a piece of sandpaper. They can be used as a wavefront marker to measure the refraction of the beam induced by a sample, which translates into a displacement of the speckle pattern. Simultaneously, a transmission and small-angle scattering signal can be obtained. Due to their compatibility with polychromatic X-rays [4] speckle-based techniques have successfully been translated to lab sources [5] making them easily accessible. Up until recently, acquisition methods had to compromise either on the achievable spatial resolution, in single-shot mode, or on scan times and the ease of setup and analysis, in scanning mode. In the last months, ways for simplifying the experimental setup and requirements have been explored by testing more general schemes for stepping the phase modulator [6].

Here, we propose a new acquisition and analysis method, for which the conditions on the arrangement, number and spacing of stepping positions are relaxed compared to other scanning modes. This allows the use of less precise, less costly scanning motors and shorter scan times while delivering high-resolution, high-contrast images, see Fig. 1.

The high flexibility to tune spatial resolution and number of steps and the applicability to different reference patterns used as wavefront markers make this approach a very versatile method that can easily be adapted to different requirements and conditions.

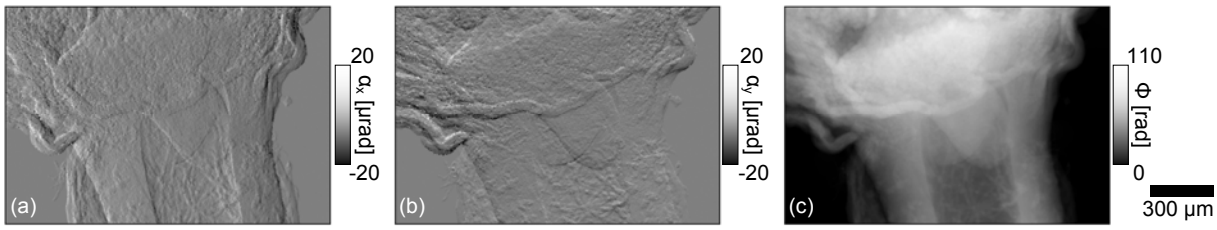

Figure 1: Refraction angle in horizontal (a) and vertical (b) direction and retrieved phase shift (c) of the bottom part of a small flower bud obtained with the proposed speckle acquisition and analysis method.

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Coherent Diffractive Imaging of Thin Film Bulk Heterojunctions for Polymer Solar Cells

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ABSTRACT

A key example of the development of cost-effective photovoltaic technologies is bulk heterojunction (BHJ) polymer solar cells consisting of a thin film fabricated by blending an electron donor polymer with a fullerene based electron acceptor.[1-2] These organic thin films offer considerable promise for the development of light-weight and flexible polymer solar cells with ultrafast charge transfer characteristics for conversion of sunlight to electricity.[3] An important criterion for good energy conversion characteristics in BHJ polymer solar cells is to have a bicontinuous interpenetrating morphology. Fast scanning calorimetry (FSC) [4-5] is a novel method that allows thermal scanning rates of more than 10^4 Ks^{-1}, thus facilitating the study of *true* isothermal morphological development by eliminating the non-isothermal effects (as negligible time is spent on temperature ramping).

Here we demonstrate that the resulting variations in the thin film morphologies for different annealing schemes can be imaged by *X-ray ptychography*, [6-7] for both FSC and conventionally heat-treated thin films. These experiments successfully enable quantitative visualization of phase-segregated organic domains with spatial resolution of about 100 nm. [8-11] In addition, we discuss the connection to corroborating experiments using ultra-small angle X-ray scattering (USAXS), to scrutinize the structural evolution of phase-segregated domains at different length scales, such as - 1) the spatially aggregated structure and molecular dispersion of the fullerene phase, and 2) the intermediate-scale structures representing the intercalation of fullerene molecules in-between the polymer chains. Finally, we present the possibility of performing *in situ* X-ray ptychography experiments on thin films to obtain movies of the domain structure dynamics as function of annealing temperature.

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PLENARY SESSION

Thursday, June 9th, 2016

SESSIONS VII, VIII, IX & X

International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Thursday, June 9th, 2016

SESSION VII
XPCS

Chairperson: M. SUTTON

IT-08	Dynamics of a colloidal glass *B. Ruzicka*
OC-14	Anisotropic De Gennes narrowing in confined fluids *Y. Chushkin*
OC-15	Structure beyond pair correlations: Higher-order correlation functions for soft matter systems *F. Lehmkühler*
OC-16	Structural origin of the anomalous dynamics of metallic glasses *B. Ruta*
OC-17	New pixel array detector techniques for X-ray photon correlation spectroscopy experiments *E. M. Dufresne*

SESSION VIII
Holographic methods

Chairperson: N. JAOUEN

IT-09	Time-resolved holographic X-ray imaging of magnetic nanostructures *B. Pfau*
OC-18	Probing magnetization dynamics by time-resolved X-ray holography with extended references *F.Y. Ogrin*
OC-19	X-ray holographic imaging of magnetic domains at the Sextants beamline of the Soleil Synchrotron *H. Popescu*

SESSION IX
Methods

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IT-10 High throughput nanoscale coherent x-ray imaging
S. Marchesini

OC-20 Near field probe retrieval and imaging at partial coherence conditions
J. Hagemann

OC-21 Phase of the transmitted wave in the dynamical theory and quasi-kinematica approximation
O. Gorobtsov

SESSION X
CDI

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IT-11 Structural X-ray studies of nanostructures using Bragg CDI at the ID01 beamline
M-I. Richard

OC-22 Imaging of the quantum well in core-shell-shell nanowires
A. Davtyan

OC-23 Quantitative interior ptychographic nanotomography
M. Guizar-Sicairos

Dynamics of a Colloidal Glass

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ABSTRACT

Dynamics of complex fluids and dynamical arrest have long been the subject of intense research, due to their unusual and unexpected behaviours. In particular, one important feature addressed in the last years is the slowing down of the dynamics (aging) and the evolution from liquid (ergodic) phases to arrested (non ergodic) states (gels and/or glasses). In this context recent advances in the study of soft materials have led to a deeper knowledge of the aging dynamics, of dynamical arrest and to the discovery of new phases and states besides the ones commonly experienced in atomic or molecular systems.

Here a deep investigation of the dynamics of a colloidal glass is discussed. The system, a colloidal clay prototype of anisotropic charged colloids, shows a nontrivial aging dynamics towards multiple arrested states. In particular, through dynamical and structural measurements implying both conventional (multiangle Dynamic Light Scattering (DLS)), synchrotron (Small Angle X-ray Scattering (SAXS), X-ray Photon Correlation (XPCS)) and neutron (Neutron Spin Echo (NSE)) techniques, compared with theory and simulations (MD), we have found the existence of equilibrium gel[1] and Wigner glass[2], respectively at low and high particle concentrations. Moreover the evidence of a glass-glass transition[3], spontaneously obtained with waiting time, has shown that the dynamics of the system still evolves even in the arrested glassy state, with a corresponding change in the shape of the intensity autocorrelation functions from stretched (black curves, $\beta<1$ in Figure) to compressed (red curves, $\beta>1$ in Figure). Finally an unexpected complex dynamics with two distinct behaviours for the microscopic and structural relaxation times across the glass transition has been found[4].

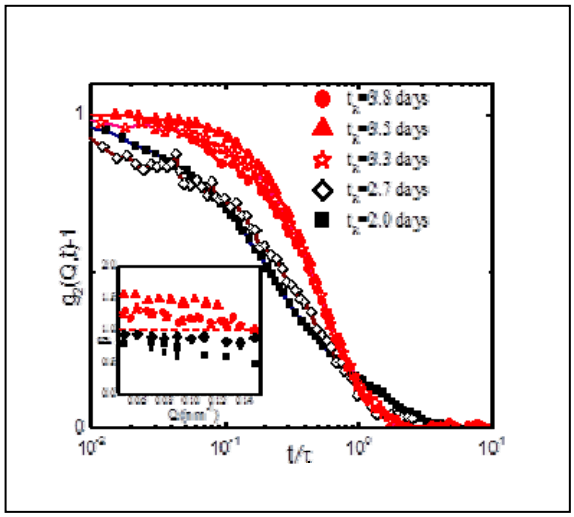

Figure: XPCS intensity autocorrelation functions for a colloidal glass at different rejuvenation times. In the inset, the β exponent is shown as a function of Q.

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Anisotropic De Gennes Narrowing in Confined Fluids

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ABSTRACT

Dense fluids in narrow spatial confinement exhibit complex microscopic ordering, due to competing packing constraints imposed by the confining surfaces and other particles in the system [1]. As a result, confinement alters the fluids' dynamic properties [2] and is thus highly relevant in a wide range of scientific phenomena and technological applications. Packing constraints in confined geometries lead to a position-dependent diffusion of dense fluids, thereby highlighting the close connection between microscopic structure and dynamics. However, a conceptually simple mechanistic picture describing complex dynamical behavior [3] in terms of the microscopic structure is still missing.

We studied the connection between the microscopic structure and dynamics of dense fluids confined between planar walls at close separation, i.e., in a narrow slit geometry by combining high-energy (21 keV) x-ray photon correlation spectroscopy and small-angle x-ray scattering from colloid-filled microfluidic channels [4]. The results show the structural relaxation in confinement to be slower compared to bulk. The collective dynamics is wave vector dependent, akin to de Gennes narrowing typically observed in bulk fluids. However, in stark contrast to bulk, the structure factor [5] and de Gennes narrowing in confinement are anisotropic. These experimental observations establish a direct connection between the structure and dynamics in confined fluids at the fundamental level of anisotropic pair densities, and thereby provide an important conceptual step towards a microscopic description of collective diffusion in dense confined fluids.

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Structure beyond Pair Correlations: Higher-order Correlation Functions for Soft Matter Systems

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ABSTRACT

Accessing structure beyond conventionally studied pair correlation functions is expected to shed light on various open questions in condensed matter physics. One prominent example is the glass transition phenomenon. Upon approaching this transition, the sample dynamics slows down by orders of magnitude while the static structure remains almost unchanged. In addition, relaxation phenomena become non-exponential pointing to a broad distribution of relaxation times and the existence of dynamical heterogeneities, suggested to be closely connected to spatial heterogeneities. Such spatial motifs are suggested to play a key role in the glass transition process, e.g., via geometrical frustration suppressing formation and growth of crystallites. Here, we will discuss the role of higher-order correlations from coherent X-ray scattering experiments by mean of X-ray Cross Correlation Analysis [1].

First, we will present the results from model structure simulation to demonstrate the potential of XCCA for accessing structures in amorphous systems [2]. Second, results from proof-of-principle cross-correlation studies on thin monolayer films made from colloidal microspheres studied by small-angle light scattering will be reported [3]. An extension of this approach towards nanometer spheres using a nano-focus X-ray beam demonstrates the power of a combined microscopy and cross correlation technique [4]. In this way preferred local structures in colloidal films upon drying and typical sizes of locally ordered regions were revealed. Third, we will show the impact of cross-correlation functions to study three-dimensional colloidal crystals with special emphasis on the detection of the crystal structure [5] and quantitative determination of structure formation upon increasing the pressure [6]. Finally, we will discuss our cross-correlation results from hard sphere colloids at various volume fractions. We observe increasing medium-range order in the glassy state and appearance of ordered clusters prior to the glass transition and crystallization. Both observations are characterized by a correlation between increasing structural higher-order correlations and slowing down of the sample.

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Structural Origin of the Anomalous Dynamics of Metallic Glasses

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ABSTRACT

Metallic glasses display outstanding thermal, mechanical and chemical properties, which make them forefront−materials for technological applications in many diverse fields such as medicine, environmental science and engineering. Their widespread use is, however, limited by their lack of stability over time due to ongoing relaxation processes and physical aging [1]. By combining time-resolved X-ray Photon Correlation Spectroscopy (XPCS) and high energy and high resolution X-ray Diffraction (XRD) we have directly connected microscopic structural mechanisms [2] and atomic motion [3,4] in metallic glasses, providing a unique broader view of their complexity at the atomic level [5].

We will show here that the atomic scale is dominated by the interplay between stress releasing rearrangements leading to density inhomogeneity annihilation and fast dynamical regimes of aging and medium range ordering processes, not affecting density, related to a more localised atomic motion. The evolution between these regimes is probably associated with a ductile to brittle transition. Our study reports also the observation of the thermal activation of a surprising secondary relaxation, which we associate to the onset of a crystallization process.

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New Pixel Array Detector Techniques for X-ray Photon Correlation Spectroscopy Experiments

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ABSTRACT

Pixel Array Detectors (PADs) have truly revolutionized x-ray experiments at synchrotrons. Because of the high spatial resolution needed to detect speckle patterns, X-ray Photon Correlation Spectroscopy (XPCS) experiments have mainly used Charge-Coupled Device (CCD) detectors with deep depletion Si sensors. Recently, PADs have shown their promise to outperform CCDs in these experiments in terms of speed, as well as per-pixel signal processing capabilities. This presentation will show some recent results demonstrating new XPCS methods using novel features of PADs [1-3]. We have, for example, extended XPCS beyond the continuous frame rate limit by using a PAD which can acquire two speckle patterns with a time delay much shorter than the average frame pair rate [1]. We have also demonstrated the performance of the Vertically Integrated Photon Imaging Chip (VIPIC) PAD that outputs a sparse data format (i.e. time stamp and two dimensional location of the absorbed x-rays) and thus can collect speckle patterns continuously with a time resolution of 6.5 MHz [2]. Finally, we present some recent XPCS results obtained with a novel dual counter dead-time free PAD with a frame rate of 12 kHz [3]. These examples, as well as worldwide efforts in PAD development promise a bright future for XPCS with today' synchrotrons, and the much brighter Multibend Achromat fourth generation sources.

These experiments were performed at beamline 8-ID-I of the Advanced Photon Source. Use of the Advanced Photon Source, an Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory, was supported by the US DOE under contract No. DE-AC02-06CH11357.

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Time-resolved Holographic X-ray Imaging of Magnetic Nanostructures

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ABSTRACT

In the last decade, soft-X-ray holography particularly found application in nanoscale imaging of magnetic samples [1,2]. As image contrast, the magnetic dichroism in the absorption of circularly polarized X-rays (XMCD effect) is exploited that allows to element-selectively probe different constituents, e.g., different layers, of the sample. Due to the integration of the X-ray holography optics and the sample into a single compact unit, the imaging process is inherently drift-free and the samples can be readily investigated under different environmental conditions such as magnetic field or temperature [3].

The high stability of the imaging process is particularly crucial for time-resolved measurements where it is possible to track the spatial reorientation of spins after excitation with an accuracy better than the spatial resolution of the images. Here, I will present examples of picosecond and femtosecond magnetization dynamics investigated using timing-modes at synchrotron radiation sources [4] as well as fs XUV pulses delivered by free-electron laser sources [5].

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Probing Magnetization Dynamics by Time-resolved X-ray Holography with Extended References

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ABSTRACT

Vortex closure domains are fascinating nanoscopic magnetic structures. As well as being exemplary model objects – in many ways the vortices behave like classical harmonic oscillators – they are versatile elementary components, which can perform a number of functions ranging from non-volatile high-density data storage to microwave generation [1-3]. Here we demonstrate our recent studies of vortex structures in thin film permalloy elements and single layer spin transfer oscillator (SL-STO) [4] using a recently developed time-resolved soft x-ray imaging technique HERALDO [5-6], which can provide high spatial resolution as well as a high level of immunity to mechanical and thermal drifts. In particular, we imaged the magnetic states of nano-contact SL-STO produced by the applied DC current. The experiments were performed at the beamline SEXTANTS, where spatial resolution down to 15 nm could be achieved. The results showed that at currents above 20 mA a magnetic contrast indicative of vortex formation could be observed. The vortex chirality correlated with the current polarity. As well as the vortex structure a magnetic contrast coinciding with the rim of the aperture was also observed. We speculate that both types of contrast are related to the effect of the Oersted field generated by the current.

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X-ray Holographic Imaging of Magnetic Domains at the Sextants Beamline of the Soleil Synchrotron

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ABSTRACT

Resonant scattering of polarized coherent x-rays offers the possibility of achieving x-ray imaging with element selectivity and magnetic sensitivity. In particular Fourier transform holography (FTH) is a lensless imaging technique [1] combining high spatial resolution, chemical selectivity and flexible sample environment. It makes use of a holographic mask, consisting of an object aperture and of one or more reference apertures, placed in front of a transparent sample. Holographic imaging relies on the interference between coherent beams scattered by the object and by the references. In the integrated mask/sample approach (were the sample and the holographic mask are deposited on the same silicon nitride membrane), the alignment is easy and the system is not affected by vibrations or drifts. The disadvantage is a complex sample fabrication and, especially, a fixed field of view. Another approach is to prepare the mask and the sample on two separate membranes: this requires precise alignment and stability, but allows for a movable field of view. We have implemented both approaches in our experimental setup. The scattered intensity is collected using a CCD camera equipped with a light-tight Al filter and a movable beam-stop. Magnetic images can be obtained using either circular or linear polarization [2]. In addition to continuous films, we analyzed the magnetic domain structure in laterally confined sub-micron objects. We used normal transmission geometry for imaging out of plane magnetic domains, while the sample was tilted by 30° [3] or 45° [4] for analyzing in-plane domains. Time resolved magnetic imaging was recently perfomed by RF pumping [5]. The IRMA2 [6] and the COMET [7] experimental stations of the Sextants beamline [8], adapted to coherent diffraction experiments in reflectivity and transmission, are already opened for SOLEIL users.

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High Throughput Nanoscale Coherent X-ray Imaging

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ABSTRACT

With ever brighter light sources, fast parallel detectors, and advances in phase retrieval methods, one can quickly turn ``imaging by diffraction'' experiments into sharp images. Here, we describe a set of experimental[1], algorithmic and [computational [2-4] methodologies, aimed at high throughput and resolution for the coming diffraction limited light source era.Together, these advances will allow rapid images across a range of macroscopic dimensions, through different energies, and time evolution at x-ray wavelength resolution.

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Near Field Probe Retrieval and Imaging at Partial Coherence Conditions

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ABSTRACT

In X-ray near field imaging experiments the probe determines the imaging quality in terms of resolution and artifacts. Distortions in the probe from optical elements placed in the beam's paths can easily spoil quantitative contrast. The conventionally applied flat field correction is in general flawed [1] and can degrade the object reconstruction.

In this contribution a full reconstruction of the probe based on multi-plane measurements of near field diffraction patterns. We implement a demonstration of the method using an example of a X-ray focusing system in Kirkpatrick-Baez geometry. The setup is located at Petra III (DESY, Hamburg) beam line P10.

In particular we show two reconstruction schemes [2, 3], generating diversity in the measurements to overcome the phase problem. The first scheme – near field ptychography (NFP) – extends the well known approach of far field ptychography to the near field case. Thus NFP requires an additional object. The object is used for probing the probe at several defocus distances in combination with a transversal scan. The second scheme – multiple magnitude projections (MMP) – relies only on longitudinal displacements of the detector. Both schemes yield results in good agreement for the reconstructed focus in shape and width. Also we can illustrate the advantage for object reconstructions, since inconsistencies normally arising from flat field division can now be accounted to the probe. Further we will show that the near-field reconstruction methods based on multi-plane recordings can be extended to the case of partial coherence. By numerical simulations and a suitable representation of modes, we show how to take into account partial spatial coherence, both in image formation and in reconstruction.

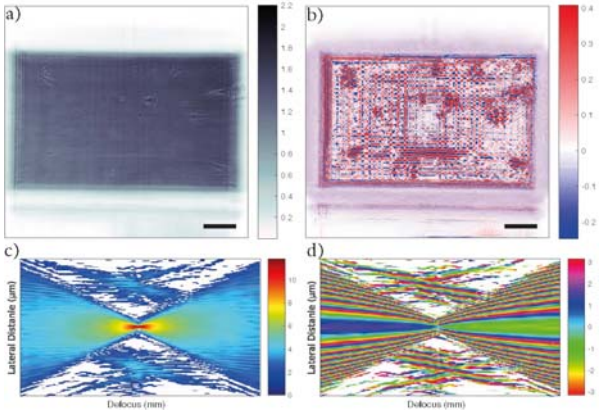

Fig. 1. Example for probe reconstruction using MMP. a) and b) show the recovered probe at the detector in amplitude and phase, respectively. c) and d) show a propagation profile in intensity and phase, respectively, around the focal plane for the vertical direction.

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Phase of the Transmitted Wave in the Dynamical Theory and Quasi-kinematical Approximation

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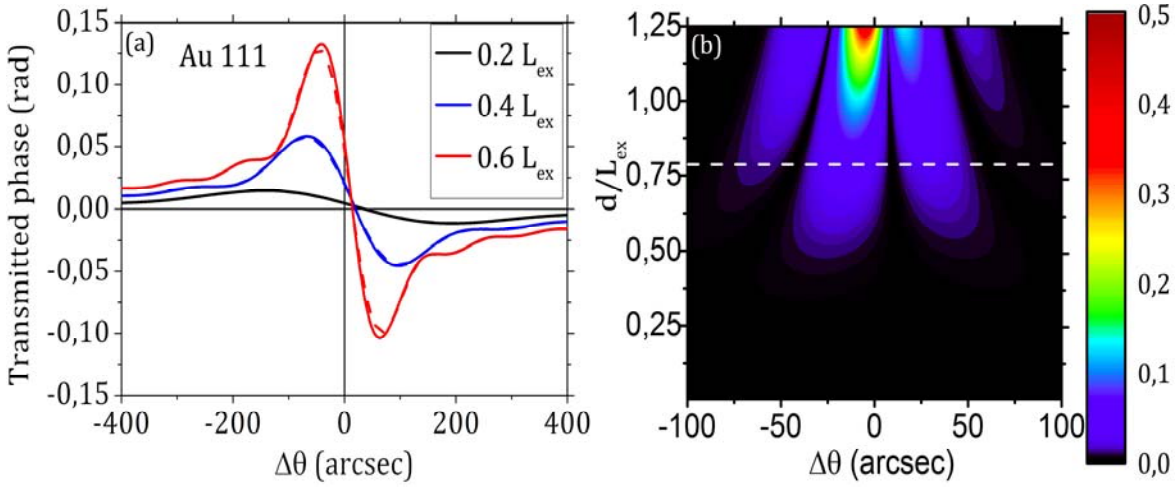
ABSTRACT

Variation of the phase of the beam transmitted through a crystalline material as a function of the rocking angle is a well-known dynamical effect in x-ray scattering. Unfortunately, these phase variations cannot be easily measured in a conventional scattering experiment. It was recently suggested[1] that the transmitted phase can be determined in ptychography experiments performed on nanocrystal samples. Results of such experiments for different crystal thickness, reflections and incoming photon energies can in principle be fully described in the frame of dynamical theory. However, dynamical theory does not provide a simple analytical expression for further analysis.

We have developed a quasi-kinematical theory approach[2] that allows to describe correctly and in a simple way the phase of the transmitted beam for the crystal thickness less than extinction length that is beyond applicability of the conventional kinematical theory. The possible implications of the described transmitted phase variation for ptychographical experiments on nanocrystals are considered. Fig., (a) shows comparison between dynamical (solid) and quasi-kinematical (dashed) expressions for transmitted phase as a function of rocking angle. Fig., (b) shows the relative error of quasi-kinematical approximation depending on crystal thickness.



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Structural X-ray Studies of Nanostructures using Bragg CDI at the ID01 Beamline

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ABSTRACT

Characterizing the structural properties (strain gradients, chemical composition, crystal orientation, defects, …) inside nanostructures is a grand challenge in materials science. This contribution will illustrate how Bragg Coherent Diffraction Imaging (Bragg CDI) can be utilized to address this challenge for crystalline nanostructures at the upgraded ID01 beamline of the European Synchrotron Radiation Facility (ESRF). Coherent reconstruction can be used at ID01 to resolve strain and structure in three dimensions. The spatial resolution depends on the data quality and is determined by the coherent flux and ultimately limited by the wavelength. A resolution of the structural properties of less than 10 nm is achieved up-to-date for Bragg CDI at ID01.[1] In the near future more brilliant X-ray sources (*e.g.* after the ESRF EBS (Extremely Brilliant Source) Upgrade scheduled in 2018/2019) will provide significant gains in coherent photon flux and opens exciting perspectives by pushing down the spatial resolution.

Here, the capabilities of the Bragg CDI technique will be demonstrated on two types of single and isolated nanostructures: functionalized core-shell nanowires[2] and highly faceted metallic nanoparticles for enhanced catalysis. The control of interfaces and surfaces in nanostructures with high surface area to volume ratio is increasingly important in numerous nanotechnologies applied in *e.g.* catalysis and in microelectronics (nanosensors), photonic and optical devices. Both surface and interfacial structures are considered as the influencing factors on the catalytic performances of nanocrystal catalysts[3] and on the enhanced emission efficiency of core-shell heterostructures at the nanoscale[4]. We will first show that the Bragg CDI technique allows understanding the interplay between shape, size, strain, faceting, composition and defects at the nanoscale on these two types of nanostructures. We will then demonstrate that this technique opens pathways to investigate *in situ* and operando the internal structural evolution of nanoparticles in various gaseous and liquid environments during reaction.

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Imaging of the Quantum Well in Core-shell-shell Nanowires

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ABSTRACT

Current progress in growing nanoscale materials like nanotubes or nanowires enables to form fundamentally new building blocks for advanced types of transistor devices. In this work we investigate the structure of individual inorganic semiconductor core-shell-shell nanowires by means of Bragg coherent X-ray diffraction (BCXD). In particular BCXD measurements have been performed using GaAs/InGaAs/GaAs heterostructure nanowires with 140nm GaAs core-10nm $In_{0.15}Ga_{0.85}As$ quantum well-30nm GaAs outer shell at beamline ID01 at European Synchrotron Radiation Facility (ESRF). A coherent X-ray beam, focussed down to 150x250nm^2 (FWHM) was used to probe different wires grown on the same patterned silicon substrate by recording 3D reciprocal space maps around the (333) Bragg peak (fig.1). Due to the small beamsize only a segment of the wire was illuminated. In order to retrieve the hexagonal shape of the nanowire the 3D diffraction pattern were integrated along q_z direction and served as input for the phase retrieval algorithm. The reconstructed 2D phase pattern shows an inhomogeneous phase distribution with anomalies at the corners of the nanowire (red and yellow spots in fig. 2). Due to the elaborate variation of the diffraction intensity along q_z (see fig. 1b) more information about the structure of the wire along the growth direction can be obtained by reconstructing the 3D distribution of amplitudes and phases of the measured segment. Considering preliminary results of 3D phase retrieval (not shown here) we explain the BCXD pattern by small wurtzite segment that has been incorporated between two zinc-blende segments along the nanowire growth direction. We attempt to show that the 3D phase retrieval will reveal the phase and amplitude information along all three directions in real space.

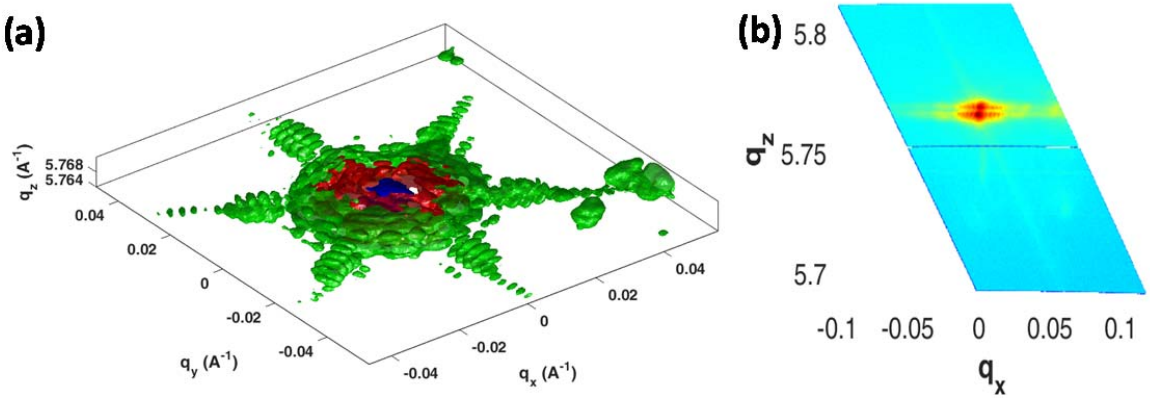

Figure 1. (a) 3D reciprocal space may around the (333) GaAs from single GaAs/InGaAs/GaAs wire. (b) Reciprocal space map integrated along the q_y direction.

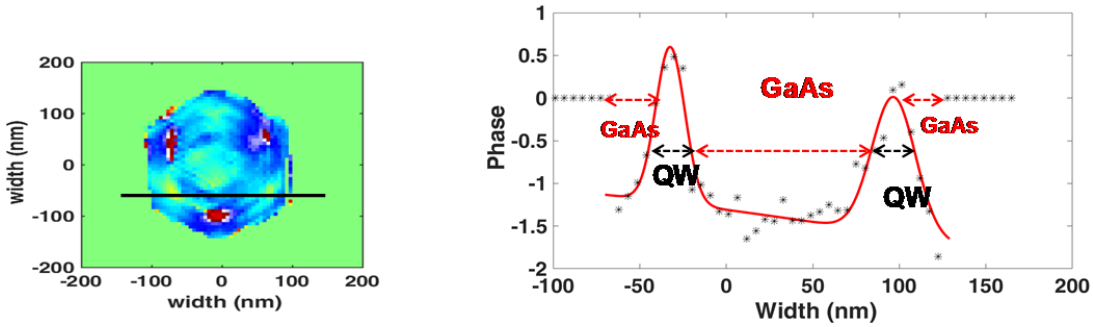

Figure 2. (left) Reconstructed phase in real space. (right) line cut along the corners of the nanowire showing the phase change at the expected position of InGaAs shell.

Quantitative Interior Ptychographic Nanotomography

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ABSTRACT

Biological and artificial materials hinge on hierarchical structures for improved mechanical performance. Understanding and modeling their macroscopical mechanical properties require characterization methods addressing length scales and resolutions that span multiple orders of magnitude. Accordingly, the capability of zooming into a region of interest within the sample is ubiquitous in 2D imaging and provides context to the smaller examined region.

For computed tomography the capability to zoom into a region of interest requires reconstructing the 3D image from truncated or interior projections, a problem that is known to be ill-posed [1]. If conventional reconstruction algorithms such as filtered back projection are used, the resulting image can present artifacts and the quantitativeness of reconstructed values is lost.

We will present methods that enable interior quantitative reconstructions for ptychographic X-ray computed tomography (PXCT) [2] by combination of nanoscale-resolution interior projections with coarser quality measurements [3,4]. Thus allowing the possibility of zooming into 3D regions of interest within the sample, which allows for more efficient use of measurement time and simplifies sample preparation.

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PLENARY SESSION

Friday, June 10th, 2016

SESSIONS XI & XII

International Workshop on Phase Retrieval and Coherent Scattering

COHERENCE-2016

Friday, June 10th

SESSION XI
CDI

Chairperson: O. THOMAS

IT-12	Frontiers of X-ray science developed with coherent X-rays of SACLA *M. Yabashi*
OC-24	Massive faulting of gold nanocrystals upon alloying with iron *A. K. Estandarte*
OC-25	On the origin of biomimetic $CaCO_3$ complex morphologies *T. Beuvier*
OC-26	X-ray coherent diffractive imaging of defects in bio-photonic crystals inside butterfly wing scales *A. Singer*
OC-27	Coherent Bragg imaging of crystal defects during in situ indentation *M. Dupraz*

SESSION XII
Ptychography

Chairperson: F. BERENGUER

IT-13	Applications of X-ray ptychography at the Swiss Light Source *A. Diaz*
OC-28	X-ray ptychography: Fast, cold, colorful, and sharp *C. Jacobsen*
OC-29	Dark-field X-ray ptychography: High-resolution imaging of weak-phase objects *N. Burdet*

Frontiers of X-ray Science Developed with Coherent X-rays of SACLA

M. Yabashi

RIKEN SPring-8 Center

ABSTRACT

As the first compact XFEL facility, SACLA has operated for users since its inauguration in March 2012. SACLA has routinely generated XFEL light in a photon energy range from 4 to 15 keV with a pulse energy of ~0.5 mJ at 10 keV and a pulse duration less than 10 fs[1], which corresponds to a high peak power of several tens gigawatts. SACLA can optionally produce two-color SASE XFEL light with a large separation of the two wavelengths over 30% by using variable-gap, in-vacuum undulators[2].

To enhance capabilities, we have developed various X-ray optical systems[3,4] and experimental platforms. One of the key devices is X-ray focusing optics, in particular, a two-stage focusing system, which generates an extremely high intensity of 1e20 W/cm^2 by forming a 50-nm spot[7]. We have utilized this ultraintense X-ray beam to explore unique researches in a field of quantum/non-linear x-ray optics, such as achievement of Cu Kα atomic laser[8].

Another key requirement is expansion of capacities for enlarging experimental opportunities of XFEL sources. For this purpose, we have developed a 2nd hard X-ray FEL beamline (BL2) and a soft X-ray FEL beamline (BL1), in addition to the existing XFEL beamline (BL3). In this talk, I will give the latest status, typical experimental achievements[9], and future plans of SACLA.

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Massive Faulting of Gold Nanocrystals upon Alloying with Iron

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ABSTRACT

Bragg Coherent Diffraction Imaging (BCDI) was used to investigate the alloying of Fe and Au in an in situ experiment at the Diamond Light Source I-07 beamline for surface diffraction. Preformed 300 nm diameter Au nanocrystals were mounted in the Ultra-High Vacuum (UHV) diffractometer of EH2. 20 μm slits were used to illuminate a sufficiently small number of crystals that the coherent diffraction pattern of one of them could be isolated on the Pilatus detector placed 1.5 m away. After centering the crystal on every scan, the 3D BCDI data were measured as rocking scans, oversampled in all three directions. These data were inverted to images using the "Guided Hybrid Input-Output" algorithm [1]. Once the Au crystal was stable at 643 K on the heater stage, Fe was evaporated onto it and its evolution was followed both during and after evaporation. Rocking scans were repeated every 15 minutes during the experiment.

Time dependence was observed after the first Fe evaporation but not after the second Fe evaporation where the alloying equilibrated relatively quickly. A dramatic phase structure was observed immediately after the first evaporation. Cross sectional views of the phase before and after Fe evaporation are shown in the figure below. When this phase is interpreted as a projection of the lattice distortion in the standard way [2], it shows a very unusual pattern. Along the Q-vector, denoted by the arrow, conventional inward relaxation of the two surfaces is seen by the positive and negative phase. However, there is a cylindrically symmetric positive phase surrounding this axis, which increases radially. Our current interpretation is that there is massive faulting of the crystal due to misfit of the Fe-alloyed regions near the surface of the crystal.

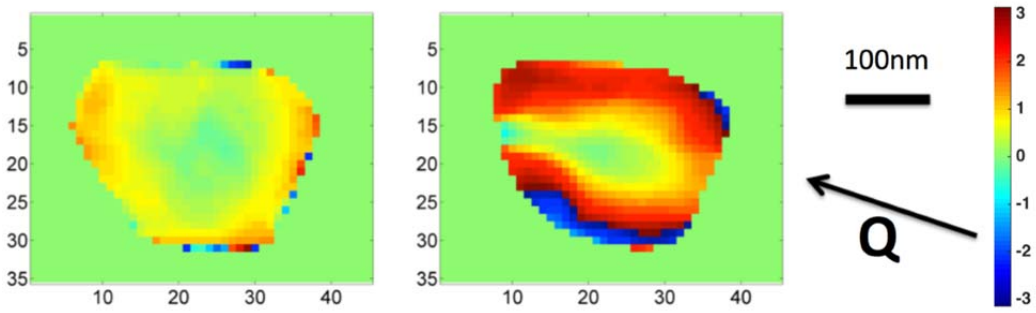

Figure 1. Phase image of the Au crystal before (left) and after (right) Fe deposition.

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On the Origin of Biomimetic $CaCO_3$ Complex Morphologies

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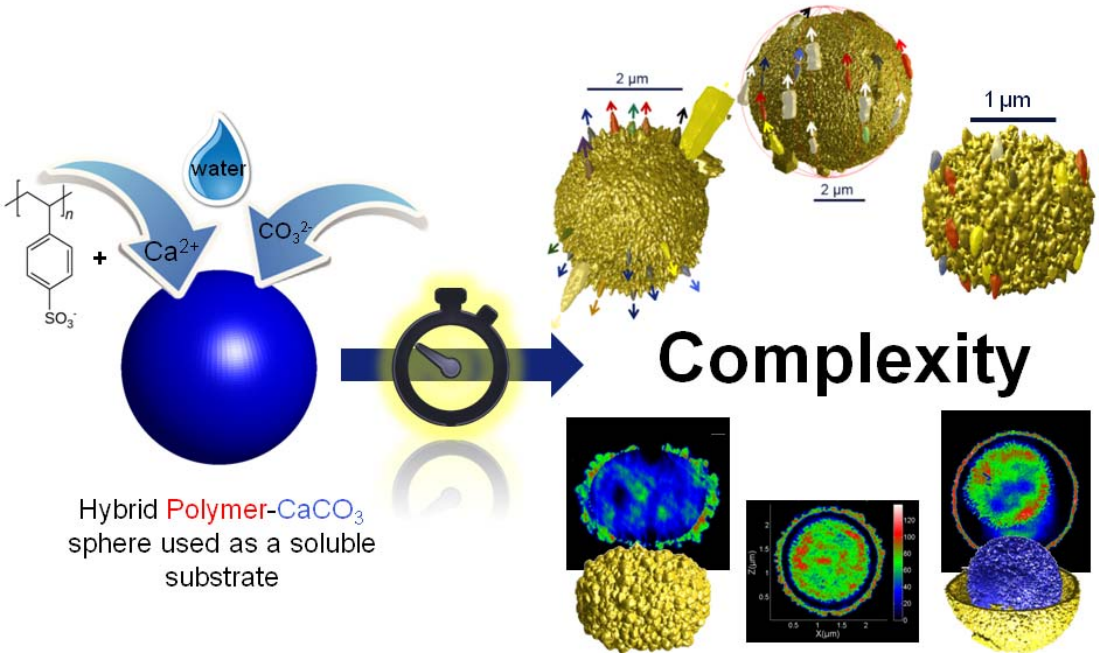
ABSTRACT

The complex architecture of biominerals arises from their interactions with macromolecules [1]. Yet, little is known about the role of these macromolecules in directing precipitation and recrystallization. Here, by using coherent X-ray diffraction imaging (CXDI) on ID10 [2], we investigate the self-transformation of biomimetic CaCO3 microparticles formed in a matrix of polystyrene sulphonate (PSS).

Through the morphological description of around 20 samples by 3 dimensional CXDI, we describe the development of the shape complexity. Notably, we discuss notably the interplay between the Ostwald ripening and the oriented self-assembly processes and propose energy minimization pathways leading to the various complex morphologies.

This study should help to better understand the formation of the complex biogenic calcium carbonate structures as the spicules of tunicates (Herdmania momus [3,4]).



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X-ray Coherent Diffractive Imaging of Defects in Bio-photonic Crystals inside Butterfly Wing Scales

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ABSTRACT

Many organisms in nature have evolved sophisticated cellular mechanisms to produce photonic nanostructures, and in recent years, diverse crystalline symmetries have been identified and related to macroscopic optical properties. However, since we know little about the distributions of domain sizes, the orientations, and the nature of defects in these structures, we are unable to make the connection between the nanostructure and its development and functionality.

Here, we report on non-destructive studies of the morphology of chitinous photonic crystals in butterfly wing scales. Using spatially and angularly resolved x-ray diffraction, we find that the domains are highly oriented with respect to the whole scale, indicating growth from scale boundaries. X-ray coherent diffraction imaging reveals two types of crystalline domain interfaces: abrupt changes between domains emerging from distinct nucleation sites and smooth transitions with edge dislocations presumably resulting from internal stresses during nanostructure development. Our study of the scale structure reveals new aspects of photonic crystal growth in butterfly wings and shows their similarity to block-copolymer materials. It opens new avenues to explore fundamental processes underlying growth of biological photonic nanostructures in a variety of species.

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Andrej Singer, Leandra Boucheron, Sebastian H. Dietze, Katharine E. Jensen, David Vine, Ian McNulty, Eric R. Dufresne, Richard O. Prum, Simon G. J. Mochrie, and Oleg G. Shpyrko (submitted 2015)

Coherent Bragg Imaging of Crystal Defects during *In Situ* Indentation

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ABSTRACT

The stochastic nature of plastic deformation becomes predominant in micro-/nano-crystals [1], and their mechanical behaviour under loading cannot be understood without an accurate knowledge of the microstructure (before and during loading). Based on the results of a recent experiment performed at ID01, we demonstrate that Coherent Bragg Imaging [2] is a valuable alternative to Transmission Electron Microscopy (which is restricted to thin samples) for the observation of the crystal microstructure during mechanical loading.
We loaded a gold microcrystal with the help of our home-made Atomic Force Microscope installed on the diffractometer [3], and imaged the crystal structure by Coherent Bragg Imaging (on the 111 Au peak) at several early stages of the indentation. The density and phase maps obtained by inverting the diffraction patterns reveal, at one stage, a dislocation loop of 50 nm diameter nucleated during loading and trapped in the crystal. The phase analysis allows the unambiguous identification of the prismatic nature of the dislocation loop [4]. In addition, a modification of the reconstructed displacement and strain fields after several loadings, as well as an evolution of the particle shape and strain field after 24h ageing under the X-ray beam are observed and discussed.

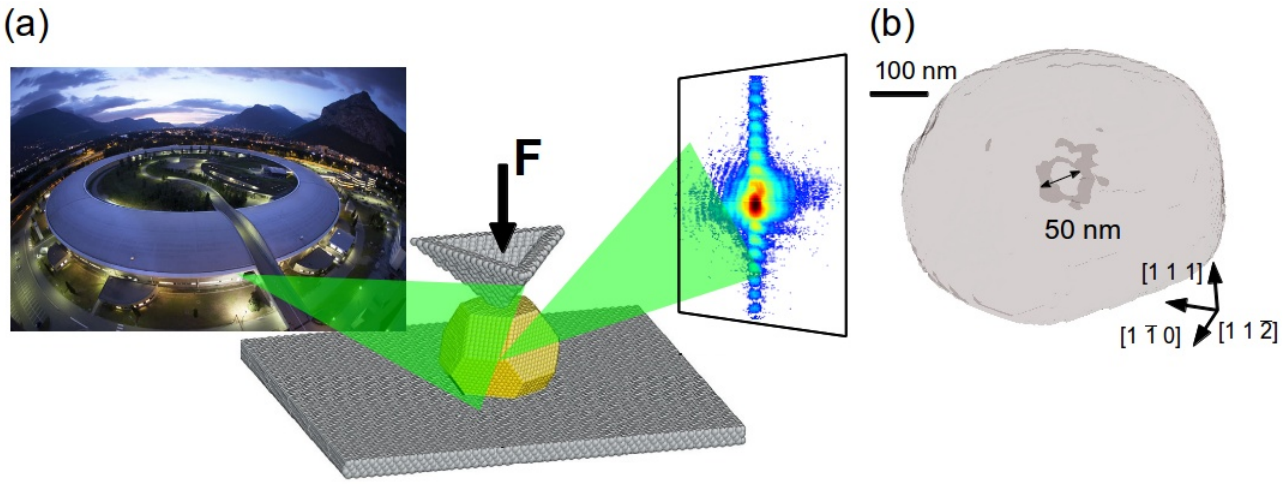

Fig. 1 (a) Schematics of the experiment and reconstructed electron density of the sample after indentation showing a prismatic loop trapped inside.

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Applications of X-ray Ptychography at the Swiss Light Source

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ABSTRACT

X-ray ptychography has been established in the last few years as a powerful imaging technique due to a combination of features such as high phase sensitivity with quantitative values, high resolution and arbitrarily large fields of view. X-ray ptychography finds useful applications in the multi-keV energy regime because of the technical difficulties to fabricate efficient X-ray lenses for these energies. Our group at the cSAXS beamline at the Swiss Light Source is devoted to implement X-ray ptychography as a tool for users. The main goal is that users from different fields of research can perform their experiments without having any expertise in the technique. In this presentation we show our latest applications of X-ray ptychography, including efforts towards in-situ experiments [1,2], high-resolution tomography [3,4] and cryo-imaging of biological specimens [5]. We will also present the developments in algorithms, data acquisition strategies and instrumentation that make these applications possible.

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X-ray Ptychography: Fast, Cold, Colorful, and Sharp

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ABSTRACT

X-ray ptychography has seen rapid development as a coherent imaging approach for extended objects, with a resolution limited by the scattering signal collected rather than by an optic. We describe our efforts to make it fast, cold, colorful, and sharp:

- We make it fast by using continuous-scan methods[1,2] which will become increasingly important at future diffraction-limited storage ring light sources, and by using a parallelized reconstruction code[3]. This is allowing us to obtain images during experiments.
- We make it cold by using specimens at cryogenic temperatures[4], where one obtains excellent preservation of structure and chemistry in biological specimens.
- We make it colorful by combining it with x-ray fluorescence[5,4], so that ptychography can be used to image cellular ultrastructure (comprised of light elements with poor fluorescence detection) and fluorescence can be used to image trace elements which are important in normal and diseased cell function.
- We make it sharp by combining the above to produce higher photon density on the specimen; this allows us to collect the signal scattered from fine, low contrast features. By obtaining two successive images of the same frozen hydrated cell, we are able to show from resolution-dependent correlation that we are able to obtain images with 18 nm resolution.

We will discuss extension of these approaches to 3D.

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Dark-field X-ray Ptychography: High-resolution Imaging of Weak-phase Objects

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ABSTRACT

Phase shift of light or electrons in objects is now necessary to probe weak-phase objects such as soft bioogical tissues. Optical microscopy (OM) and transmission electron microscopy (TEM) have been used to observe weak-phase objects such as biological specimens. However, classical OM has low spatial resolution and TEM is limited to thin specimens. While classical X-ray ptychography can accurately retrieve the phase, the large dynamic range of diffraction patterns together with the data missing behind the beamstop still represent a barrier towards further increasing the spatial resolution and sensitivity. Dark-field X-ray ptychography [1], which uses a reference light source to create an inline hologram, has been recently proposed as a means of overcoming these limitations. Figure 1 shows a schematic view of dark-field X-ray ptychography. By combining X-ray ptychography and X-ray in-line holography in an alternating phase retrieval calculation scheme, we were able to observe a test object of 30-nm-thick Ta with a phase sensitivity better than 0.01 rad, a spatial resolution better than 15 nm, and a field of view larger than 5 μm. We have applied this method to the high-resolution observation of both the shape and internal structure of magnetic bacteria MO-1. Figure 2 shows a phase image of MO-1. The ability to observe a thick sample with a high resolution and high sensitivity is expected to have broad applications in not only biology but also materials science.

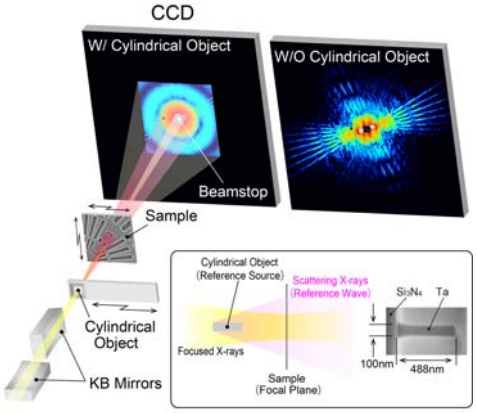

Figure 1: Schematic view of the experimental setup of dark-field X-ray ptychography.

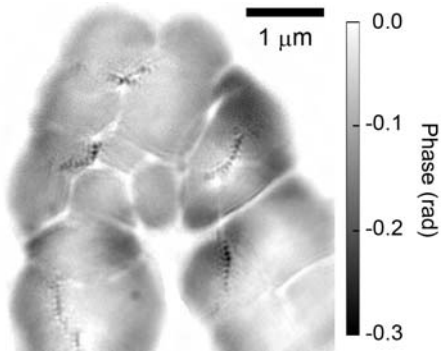

Figure 2: Reconstructed image of the magnetic bacteria MO-1.

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Coherent X-ray Diffraction of Single Epitaxial Nanodots

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ABSTRACT

The nanoparticle shape is an influential factor in many catalytic activities because it could dictate the adsorption free energy by the atomic arrangement on the catalyst surface[1]. Therefore, in order to understand the size-dependence of catalytic processes novel approaches to controlled nanocatalysis are required[2].

In this work we report on a one-to-one structure analysis of randomly deposited Ir nanodots, a single Ir nanodot and a single Pt nanodot-array, all of them grown on STO(100) single crystals[3]. Complementary information has been obtained by real-space imaging in a scanning electron microscope and in reciprocal space using coherent Bragg diffraction[4] from a focused X-ray beam at PETRA III at DESY.

The Pt nanodot-array was created using a combined lift-off and etching process based on e-beam lithography, whereas the Ir nanodots were deposited by e-beam evaporation[5]. We localized these nano-objects utilizing a transfer and repositioning protocol using the Pt X-ray fluorescence.

We propose the use of these systems for future experiments on in-situ oxidation or catalysis as well as for coherent X-ray diffraction of single nano-assemblies under reaction conditions.

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The Coherent Diffraction End-station in Beamline CRISTAL at Synchrotron SOLEIL

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ABSTRACT

The diffraction beamline CRISTAL at Synchrotron SOLEIL has developed a high-precision and high-resolution experimental setup optimized for the study of nanostructures and materials via coherent diffraction techniques. This setup has been designed in order to meet the increasing user's demands on ultra-precise and stable Bragg coherent diffraction imaging (Bragg-CDI) and Bragg ptychography measurements.

CRISTAL is located in a short straight section of the ring fed by a U20 undulator and it operates in the medium-hard X-ray energy regime (4-30 keV). The high-precision positioning setup for coherent diffraction is equipped with a set of five piezomotor-driven translations (10 nm resolution) mounted on an ultra-precise goniometer (10^{-5} degree resolution). Currently, the beam can be focalized down to 1x3 microns on the sample by using a set of Fresnel zone plates with focal lengths optimized to work between 5.9 to 10 keV. A Maxipix 2 detector (55 micron pixel size) is used for the data acquisition. An upgrade of the goniometer is planned for the future in order to include a chi cradle and a controlled atmosphere sample environment.

In this communication, we present the experimental station and show selected examples of the results obtained with this setup.

Introduction of Ptychographic Imaging at MAXYMUS X-ray Microscope

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ABSTRACT

Ptychography is a recently developed X-ray diffraction imaging technique which using phase retrieving reconstruction algorithms helps to achieve spatial resolution of few nanometers [1,2] with chemical [2] and magnetic [3] contrast sensitivity. The MAXYMUS microscope, operated by the MPI for Intelligent Systems at the Bessy II synchrotron (Berlin, Germany), has been extensively upgraded for the purposes of ptychographic imaging implementation. As a result advanced capabilities of MAXYMUS microscope for high coherence and brightness, selectable polarization of X-ray light, as well as adjustable magnetic field setup, goniometric and cryostat sample holders, synergize with high ptychographic resolution.

The main part of MAXYMUS upgrade included the acquisition of a new fast in-vacuum CCD camera developed by PNSensor [4]. This instrument allows spatial and energetically sensitive single photon detection in the soft X-ray energy range at rates up to 1000 fps (frames per second) with high quantum efficiency (>70% for E>300eV) and extremely low noise. High dynamic range and fast read out rate produce efficient representation of diffraction data during ptychographic scanning. This implementation results a significant increase in the lateral resolution taking all advantages of the soft X-ray ptychography technique.

We are going to show the results of commissioning of the new in-vacuum CCD camera and the implementation of ptychographic approaches at MAXYMUS microscope. The first ptychographic reconstructions with advanced resolution in comparison with conventional STXM imaging will be demonstrated (Figure 1).

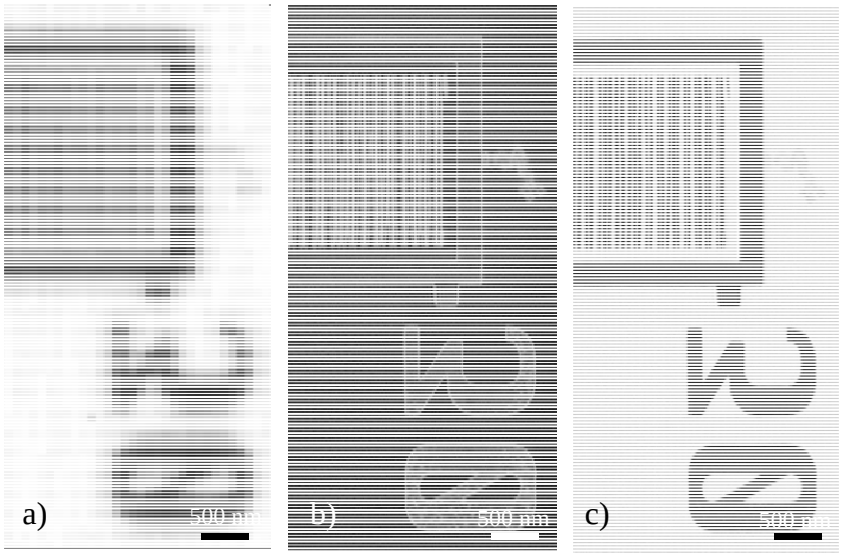

Figure 1: Resolution sample (Zeiss) with the smallest line size 30 nm imaged at energy 800 eV using high efficiency FZP with spatial resolution of 152 nm:

a) STXM image;

b) imaginary part of ptychographic reconstruction;

c) real part of ptychographic reconstruction.

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Soft X-ray Coherent Imaging at the SCS Instrument at European XFEL

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ABSTRACT

The Spectroscopy and Coherent Scattering (SCS) scientific instrument is one of the six baseline instruments of European XFEL. The SCS instrument aims to provide a diverse and complementary experimental infrastructure that takes advantage of the unique properties of the European XFEL in the soft X-ray energy range of 0.25 – 3 keV.

The instrument is focused on solid-state systems and offers a range photon-in-photon-out techniques such as small-angle X-ray scattering, coherent diffraction imaging, resonant inelastic X-ray scattering (RIXS) and X-Ray correlation spectroscopy. Along with photoemission, these can all be performed in a pump-probe configuration for femtosecond time-resolved studies.

Revealing the Meso-crystallinity Arrangement of a "Single-crystalline" Calcareous Biomineral

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ABSTRACT

The diversity of crystalline architectures observed in calcareous biominerals strongly contrasts with the consistent observation of a submicrometric granular crystalline structure [1]. Understanding how the mineral granules organize is a key element to gain knowledge on the biomineralization processes. While evidences for the existence of a mesoscale crystalline organization, spanning a few granules, have been reported, a 3D image of the spatial organization of such crystalline domains was lacking.

In this context, we have proposed to use 3D x-ray Bragg ptychography microscopy [2], an inversion based [3] coherent diffraction imaging approach, which exploits the partially redundant information obtained by scanning a finite beam spot size transversally to the sample, while measuring the corresponding 3D far-field intensity diffraction pattern. Thereby, 3D imaging of extended crystalline samples becomes possible [4, 5].

We obtained 3D images of the prismatic part of a *Pinctada margaritifera* shell, revealing this way the spatial arrangement of the crystalline structure with a nanometric resolution. We evidence a crystalline coherence extending over a few granules and further prove the existence of larger iso-oriented crystalline domains, slightly misoriented with respect to each other around a single rotation axis [6]. These original results bring new structural information, which will be discussed in the framework of recently proposed biomineralization growth schemes.

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Damage and Orientation in Single Molecule Imaging using X-ray Free Electron Lasers

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ABSTRACT

Single molecule imaging using femtosecond pulses from an x-ray free electron laser (XFEL) is a promising method for determining structures of large molecules that are inaccessible to current techniques including crystallography. In order to resolve the molecular structure, damage due to the XFEL [1-3] and the orientation of the particle [4,5] need to be considered. So far, each of these have been investigated independently, but they are rarely treated together.

Damage to biomolecules from XFEL pulses has been studied in the context of molecular dynamics [1], rate equations models [2] and electronic damage [3]. Imaging of single molecules involves injection of identical samples into a XFEL beam in random and unknown orientations. Diffraction patterns for each of the orientations are recorded and are then assembled into a three-dimensional density distribution using orientation reconstruction algorithms [4,5]. Due to the complexity of the task, these methods do not yet account for damage to the molecule.

We explore the damage caused to the molecule GroEL, a molecular chaperone, by an incident intensity of 2.0×10^{20} W/cm^2 using a rate equations model that accounts for photoionization, secondary ionization, ejected electrons and Auger decay. We have predicted that single particle diffraction with longer pulse times of up to 100 fs exhibit a self-gating effect [6], whereby the diffraction patterns at later times still contain significant information about the initial ion positions. We present results from a statistical model that uses the Pearson correlation to compare damaged and undamaged speckle contrasts. The study of the correlation function is a first step toward an analysis of the effect of damage on the performance of orientation algorithms.

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High Energy Nano-imaging at the ID16A Beamline of ESRF: Exploiting the Coherence of Hard X-rays for Better 2D and 3D Images

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ABSTRACT

X-ray imaging with coherent X-rays produced by synchrotron sources has already shown great potential for high resolution quantitative microscopy. We present here the different ways we exploit the coherence of high energy X-rays at the ID16A beamline of ESRF. The image reconstruction is enabled by adding either longitudinal diversity to the phase retrieval, in the case of in-line holography, or transverse diversity for far- and near-field ptychography. In addition, the combination with tomography makes 3D imaging possible via holographic-tomography or ptychography X-ray computed tomography. However, implementing such techniques with very high photon flux and high energies is challenging. The main difficulties arise from the degradation of the experimental conditions and shortcomings of current detector technology. Typically, the increase of photon flux is obtained at the expense of a large bandwidth provided by multilayer mirrors, which reduces the amount of spatial and spectral filtering and deteriorates the coherence properties of the beam. In addition, the higher the photon energy, the more difficult to obtain a reasonable degree of transverse coherence of the beam, which requires building the endstation at a long distance from the source. Furthermore, the available technologies of X-ray detection systems are not yet optimized for high energy and high photon flux, forcing us to work with limited dynamic range and unwanted background. We will show how we have tackled these challenges in order to make high quality and high resolution 2D and 3D imaging at the nanoscale possible. The most recent algorithm developments enable us to circumvent the non-ideal experimental conditions and allow broad bandwidth coherent X-ray imaging. In addition, the high energy photons and small nanofocus allow the combination of coherent imaging with X-ray fluorescence analysis by exciting important high Z elements such as Fe or Au (Fig. 1). Finally, we will show the latest developments in coherent X-ray nano-imaging implemented at our beamline and important applications to materials science.

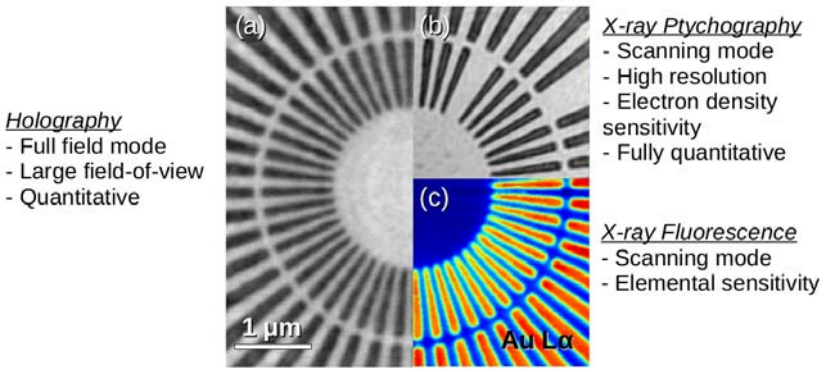

Figure 1: The techniques available at ID16A Nano-Imaging beamline, ESRF, applied to a 200 nm thick “Siemens Star” made of gold. (a) Holography. (b) Ptychography. (c) Fluorescence imaging.

Angular Scattering of Polarized E.M. Radiation Techniques, LS vs SAXS, Applied to Probe the NPs Born in the Gas Phase whatever their Absorption Nature

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ABSTRACT

In the everyday life (e.g., cooking, gardening, photography, etc.) it is quite evident that *different* working tools (e.g., spoon, mixer, sieve, etc) do serve to perform *different* jobs. *Not* so evident in science. Very often the researchers are induced to the mental aptitude to consider their findings as absolute evidence independently from the diagnostic techniques used in the experiments.

Flame soot NanoParticles (NPs) aggregates, and their hierarchical “DNA-genomics” proved in the last 15 years by our group (di Stasio,2001; di stasio et al, 2006), is a fantastic example, in which if one performs the experiments by different techniques, he/she will gain different but complementary information (if and only if the experiments are correctly conceived and performed and data are correctly processed). With particular regard to the scattering techniques, the meter of the magnifying lens with which you look at NPs aggregates is given by the wavelength λ of the e.m. radiation that is used. As a rule-of-thumb, light scattering is useful in the experiments if NPs are larger than about $\lambda/10$, i.e., with the best (laser) light sources and the best detectors you have no hope to detect NPs and/or agglomerates below an overall size about 15 to 40 nm. Vice versa, the wavelength of soft X-ray (about 10 keV energy) is usually below 1 Å, which returns in SAXS/WAXS/GISAXS experiments a quite complementary information on NP clusters. In the case of flame soot NPs clusters it is observed either from SEM/TEM analysis and by SAXS and Light Scattering results, that within such aggregates one can distinguish primary, sub-primary and nuclei sub-units, which contribute as building bricks to the formation of upper level size nanostructures (biblio).

This talk makes focus on the fact that the Talmud-like (*) observation of NP aggregates, whatever their nature (both absorption or not-absorption species), by using both *in-situ* (LS, SAXS) or *ex-situ* (XRD, SEM/TEM, ADB, UV-VIS and FTIR Spectroscopy) techniques, it is a powerful aptitude of mind for the investigators, who can change the “lens of observation” and really touch the PROs and CONs of each tool and how information returned by the different techniques, if correct, is absolutely complimentary to get insight into reality. The working example will be the scattering experiments focused on flame soot NPs.

(*) we learn from this ancient book (Stemberger, 1982) that the correct way to have a look to facts or happenings is to looking at it by 33 different points of view.

Bragg Coherent X-ray Diffractive Imaging of a Single Indium Phosphide Nanowire

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ABSTRACT

Here we present the result of three-dimensional (3D) Bragg coherent x-ray diffractive imaging (CXDI) of a single indium phosphide nanowire [1]. A nanofocused x-ray beam was used as a probe. Quantitative information about strain distribution inside the nanowire was obtained by pre-characterization of the beam profile (see Fig. 1 (a)) with transmission ptychography measurement on a test sample. The 3D shape of reconstructed nanowire is shown in Fig. 1 (b). Our measurements were performed in a region 150 nm below the catalyst Au particle, located at the tip of the nanowire. We observed a gradient of the strain in the range of ±0.6% along the growth direction of the nanowire (see Fig. 1 (c, d)). The CXDI measurements show a good agreement with the results of finite element method simulations of the strain in InP nanowire. The spatial resolution of the nanowire reconstruction was about 10 nm in the direction perpendicular to the facets of the nanowire.

The proposed approach can become an effective tool for *in operando* studies of the nanowires without destructive sample preparation.

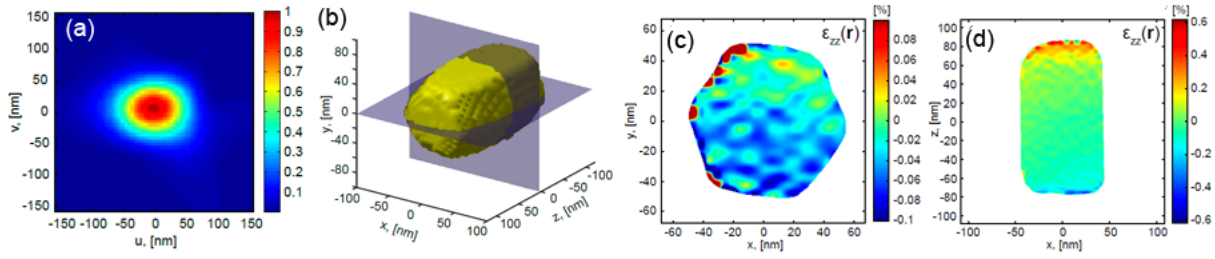

Figure 1. (a) Beam profile reconstructed by transmission ptychography; (b) Part of the nanowire in 3D reconstructed by Bragg CXDI; (c) and (d) 2D slices of strain distribution within the nanowire

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In situ Catalytic Characterization of Pt Nanoparticles by Coherent Diffraction Imaging

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ABSTRACT

In recent years, low-dimensional materials have attracted a lot of attention because of the expected influence of size on the chemical and physical properties of the nanostructure. In the case of metallic nanoparticles (NPs), shape and strain fields play a key role in the catalytic properties: it is well known that activity and selectivity strongly depend on the faceting and strain distribution of the NPs. Furthermore, structural changes can occur during reaction [1]. As structural changes may result in activation or deactivation phenomena, it is needed to perform *in situ* studies to understand possible structure-activity relationships. Thus, Bragg Coherent Diffraction Imaging (BCDI) has been applied here for the study of this type of systems, since it is non-destructive and allows access to the complete three-dimensional characterization of single nano-objects (e.g. morphology, strain fields…).

Tetrahexahedral (THH) Pt NPs, whose particular shape enhances catalytic properties [2], have been studied by BCDI at the European Synchrotron (ESRF, France). First, a complete characterization in inert atmosphere of a single particle has been performed at ID01 beamline: phase retrieval of the recorded diffraction patterns around the **200** Pt Bragg reflection yields a well facetted THH crystal whose facets have been indexed. The strain within the particle has been determined as well.

Furthermore, an *in situ* study at ID03 beamline of NPs (in controlled gas-phase environment) has been carried out. The recorded reciprocal space maps around the **200** Pt Bragg reflections on single particles consist of 24 streaks, each of them corresponding to one facet. Two particles have been followed as a function of temperature and different CO and O_2 mixtures. A qualitative evaluation of the raw data evidence facet changes under catalysis conditions is presented.

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Coherent Imaging with Polarized Probes: When to go for Vectorial?

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ABSTRACT

Although most of the coherent imaging methods use polarized beams, the formalism that is used to describe the probe-matter interaction and to solve the phase retrieval problem is usually scalar [1]. Such simplification is usually justified by the fact that polarization remains unaffected by the specimen. There exists however some cases where probe-matter interactions give rise to polarization changes. In the optical regime, well-known situations include microscopic anisotropy, which induces birefringence, and chirality, which is responsible for so-called optical activity. In the x-ray regime, polarization changes can be observed when photons are scattered in magnetic materials [2–5], depending on the spin orientations, or by specifically oriented bonds [6]. Polarization modifications carry therefore valuable information about material properties.

Recently, we have addressed the issue of probe polarization in the framework of the ptychography reconstruction problem [7]. A vectorial propagation formalism was used to derive a phase retrieval algorithm aiming at reconstructing the full polarization-related properties of an object, from measurements taken under an appropriate set of prepared and analyzed polarization states.

Here, we will discuss the application of this formalism, depending on the measurement conditions and investigated properties. Comprehensive criteria are provided, assessing whether the vectorial formalism is needed or not. Our discussion, which covers basic examples in the optical regime, will be extended to recent works aiming at revealing magnetic domains by means of x-ray coherent imaging [3–5].

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Fourier Transform Holography of Magnetic Multilayers on Back-thinned Glass Substrates

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ABSTRACT

Mask-based Fourier transform holography (FTH) [1] is a lensless, coherence-based imaging technique generating a full-field image by direct Fourier inversion of a far-field hologram. In combination with resonant scattering of soft X-rays, the approach allows for specific contrast mechanisms to be used, including chemical and magnetic contrast. Magnetic contrast based on XMCD is well established and can also be used for FTH image formation to obtain magnetization maps. In the past, we have for example determined the switching field distributions of prototype bit-patterned data storage media via FTH in resonance with 3d transition metal L-edges below 800 eV photon energy [2,3]. For this purpose, the BPM samples had to be produced on Si_3N_4 membranes in order to perform FTH studies with soft X-rays in transmission geometry.

Moving away from the constraint of Si_3N_4 membranes as substrate material we developed a procedure to fabricate thin substrates from bulk material while protecting the sample layer during the process. By a combination of plane grinding, dimple grinding and custom focused-ion-beam (FIB) milling we are capable to back-thin, e.g., glass substrates down to a thickness of a few hundred nanometers, which is sufficiently thin to serve as transmissive substrate for soft X-ray FTH imaging in transmission. In a proof-of-principle experiment we show that a PMMA protection layer of 500 nm thickness on the sample side keeps the magnetic layer-system intact while thinning down the substrate from the opposite side and subsequently applying a gold-film with the mask required for holographic imaging. We imaged the magnetic domain structure of the Co/Pt-multilayer-system on the glass substrate at different magnetic fields in comparison to the same magnetic multilayer system on silicon-nitride membranes in order to verify that the thinning process does not influence the magnetic systems properties. Obviously, this sample preparation approach is applicable.

To show the potential of the new preparation procedure we imaged a sample of a commercial hard disk drive without altering the data previously written to the disk. Using this preparation procedure soft X-ray FTH is no longer limited to model sample systems prepared on Si_3N_4 membranes, opening up to new substrate materials, such as MgO and STO e.g. for epitaxial growth, for coherent imaging applications in scientific as well as industrial research.

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In situ Experimental Setup to Study Magneto-electric Effects in a Single Nanoparticle using Bragg Coherent Diffraction Imaging

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ABSTRACT

Phase transitions in multiferroic and ferro-electric materials are of great interest for the development of spintronic devices, solar cells, catalysis, information and energy storage [1]. We report on a recently developed insitu experimental setup to study phase transitions in multiferroic nanostructures by means of Bragg coherent diffraction imaging [2-4]. By using a magneto-electric tester that is capable of providing variable waveforms of pulsed electric and magnetic field uniformly on a chosen sample's crystallographic direction, we were able to map local ferro-electric phase transitions in a single nanoparticle.

The system is composed of high precision voltage source, with internal waveform generator, current source and a set of electro magnets. The system is capable of driving the sample with electric field up to 10 GV per cm with pulse of variable shape and duration as well as simultaneously applying pulsed magnetic field of up to 0.5 T both synchronously and asynchronously. Hall effect sensors provide real-time feedback for calibration and adjustment of the magnetic field while the sample is under test.

In this talk, we will highlight the capabilities of our setup to study hundreds of ps to ms dynamics in a single magneto-electric nanonostructure under applied EM-field by means of Bragg coherent diffraction imaging. The further development of the system will allow to-synchronize the pulsed fields and arriving pulses of synchrotron radiation to increase the accessible temporal resolution of the experimental system.

This work was supported by the Department of Defense (DOD) through the Air Force Office of Scientific Research (AFOSR) under Award No. FA9550-14-1-0363. Professor Fohtung acknowledges support, in part from the LANSCE Professorship and Rosen Scholar sponsored by the National Security Education Center at Los Alamos National Laboratory under subcontract No. 257827.

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X-ray Photon Correlation Spectroscopy Studies of Oxygen Vacancy Dynamics in Complex Oxide Heterostructures

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ABSTRACT

We have recently discovered that $SrCoO_{3-\delta}$, an end member of $La_{1-x}Sr_xCoO_{3-\delta}$, a well-known correlated electron material as well as catalyst, can behave as an oxygen "sponge" [1]. As oxygen exits from the surface, δ approaches 0.5, and $SrCoO_{3-\delta}$ forms the brownmillerite phase, creating a superlattice peak from oxygen vacancy ordering. As oxygen is re-incorporated into $SrCoO_{3-\delta}$ via a surface redox reaction, the superlattice peak disappears as the perovskite phase is re-formed. The speed at which δ is varied depends on the sample temperature and the surrounding oxygen partial pressure (pO_2). While the redox behavior of such oxides has been the subject of recent interest [2-6], much concerning the kinetics and dynamics of these materials remain unknown.

Utilizing *in situ* coherent X-ray scattering at the Advanced Photon Source, we monitored speckle from epitaxial $SrCoO_{3-\delta}$ thin films grown on $SrTiO_3$(001) as oxygen was incorporated and evolved (switching the environment from O_2 to N_2) to gain insight into the dynamics of oxygen-induced phase evolution in complex oxide materials. We found that the kinetics of the brownmillerite to the perovskite phase transition could be varied from tens of minutes to several hours over a small temperature range (300°C to 350°C), observing pronounced differences between the oxidation and reduction behaviors, the latter involving substantial incubation times to re-nucleate the brownmillerite phase. From X-ray photon correlation spectroscopy on the brownmillerite superlattice reflection, we find that the two-time correlation function shows dynamics consistent with the redox kinetics. We will discuss the kinetics and dynamics of the vacancy-ordering phase transition and the methods used to distinguish the different atomic and electronic mechanisms taking place.

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New Directions in *In Situ* X-ray Studies of Vapor Phase Crystal Growth

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ABSTRACT

In-situ x-ray scattering using incoherent x-ray sources has proven to be a revealing tool to investigate the mechanisms of crystal and epitaxial film growth at the atomic scale.[1,2] X-ray capabilities are being rapidly improved with the development of powerful data analysis algorithms, efficient high-resolution x-ray optics, and high performance x-ray detectors. The next generation of x-ray sources will have sufficient brightness that coherent x-ray techniques will become routine. For nanodiffraction measurements, a far higher flux will be available in a diffraction-limited spot, so that techniques currently applied on millimeter regions will be done on sub-micron regions. The increased brightness will enable the application of coherent scattering techniques to real-time analysis of crystal growth. X-ray photon correlation spectroscopy (XPCS)[3] will reveal dynamics about subtle rearrangements of the crystal (e.g. motion of a step on a surface) not normally observed with other techniques. Coherent diffraction imaging will allow real-space images to be constructed from coherent speckle patterns.[4] These new capabilities open up new opportunities to explore fundamental and applied aspects of crystal growth.

To explore the impact of these emerging capabilities on crystal growth problems, we have constructed a next generation organometallic vapor phase epitaxy (OMVPE) growth system at the Advanced Photon Source. The key instrument is a six-circle diffractometer that includes a two-dimensional x-ray detector and long sample-to-detector distance needed for coherent x-ray studies. The sample goniometer incorporates a large hexapod that can precisely support and position a variety of chambers for different materials and processes. Our OMVPE growth chamber provides for heating samples to 1200C in chemically active precursor flows while maintaining sub-micron positional stability and full sample rotation. The growth system has a computer-controlled gas handling system to safely and accurately control, mix and monitor the vapor phase reactants. All diffractometer motions, and the reactant and carrier gas flows through the growth system, are interfaced using EPICS[5] servers to enable fast, flexible and customizable measurement of growth processes.

We will present initial x-ray results characterizing this system including microdiffraction studies of surface features on patterned substrates, and initial XPCS studies of atomic step dynamics at high temperature in the OMVPE environment.

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Cellular Ptychography Enhanced by NanoLabeling with Chemical Contrast at the Fe L-Edge

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ABSTRACT

Ptychograpic CDI is an adaptation of plane-wave CDI that can be used to image extended objects with high resolution by scanning a focused X-ray beam across overlapping regions of a sample and inverting their far-field diffraction[1,2],. Ptychographic CDI provides both phase and absorption contrast images of biological specimens in fixed or frozen-hydrated states[3,4]. When ptychographic CDI is performed near element-specific absorption edges, in the soft X-ray regime, it provides element-specific contrast[5].

Exploiting this phenomenon, we performed ptychograpic CDI with 710eV X-rays (the Fe L-edge) at beamline 5.3.2.1 of the Advanced Light Source, to demonstrate sensitive detection of 72 ± 4 nm sized particles composed of a 22 ± 3 nm magnetic Fe_3O_4 core encased by a mesoporous SiO_3 shell present within the fixed lamellar structure of a mammalian cell. Absorption contrast images reveal the dense iron cores of the particles engulfed by the leading edge of the cell. Phase contrast images reveal the presence of particle cores in two states, one phase shifted with respect to the other, indicating a chemical transition between iron oxidation states occurs in a subset of the particles. The high resolution achieved by the experiment, approximately 16.5 nm in 2D, produces sharp images with strong chemical contrast in a cellular context. This Fe-based chemical contrast remains present across multiple projections from the same object, ensuring that it is intrinsic to the sample and not introduced by the reconstruction process.

The use of chemical nano-probes as contrast labels within living systems is an important step toward specific labeling of biological target structures in future efforts aimed at high-resolution structure determination from thick, extended, weakly-scattering samples, including intact mammalian cells.

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On the Investigation of Calcium Carbonate Coccospheres by X-ray Coherent Diffraction Imaging

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ABSTRACT

Porous calcium carbonate particles are attracting large attention wide world due to their biocompatibility and possibility to be used in drug delivery. Such particles can be synthesized by direct precipitation or by using different organic templates and/or additives. In nature, they are most of the time produced via the use of biomolecules that direct the formation of a specific polymorph. Here we show how it is possible to analyze the morphology of Coccospheres. Coccospheres are produced by coccolitophores that are one-celled marine phytoplankton that inhabit the upper layers of coastal waters and the open ocean. Coccolithophores are the primary calcite producers in the ocean, constructing elaborate calcite plates or liths. Recent studies indicate that rising pH levels associated with increased oceanic carbon dioxide uptake may imperil coccolithophore species in the future. One expects that a doubling of present-day concentrations of carbon dioxide could result in a 20 to 40 percent reduction in biogenic calcification of coccolithophores, resulting in malformed calcareous plates and layers of plates. We show in an unprecedented way how CXDI can unveil the shape of these wonderful objects and how it can be further used to monitor the mass of coccoliths.

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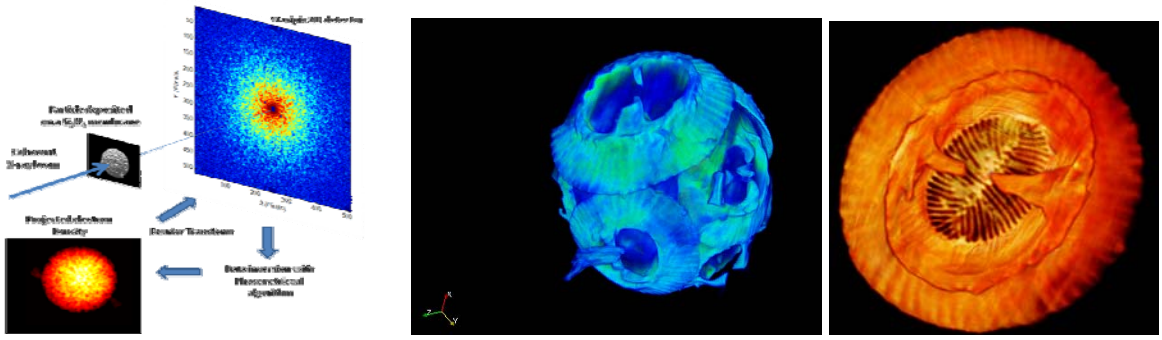

Figure 1 : left panel Sketch of the CXDI set-up showing the different steps necessary to obtain the reconstructed image of the scattering particle. Right panel : 3D image of a coccopshere and of a coccolith

Experimental 3D Coherent X-ray Diffractive Imaging from Photon-sparse Random Projections

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ABSTRACT

Single Particle Imaging (SPI) at X-ray Free Electron Laser Sources requires collection of hundreds of thousands of diffraction patterns from a continuous stream of reproducible particles [1]. As the particles arrive at the interaction region in random 3D orientations, the 3D intensity has to be assembled in Fourier space from the typically very noisy patterns, before the phasing step can be performed to obtain the real-space structure.

In order to advance XFEL-based SPI to the resolution level required to solve the structure of biological macromolecules, a great variety of experimental and algorithmic challenges have to be overcome, such as sample injection, experimental background minimization, identification of hits, orientation determination, and density reconstruction [2]. Despite many recent advances, an experimental demonstration for orientation determination of SPI data in the very relevant weak scattering limit (<~100 scattered photons per pattern) is still outstanding.

We report here on an experiment at a synchrotron source in which a small (<1 μm) lithographically produced particle has been illuminated with a coherent synchrotron beam. This way, hundreds of thousands of very weak diffraction patterns in hundreds of particle orientations have been collected.

We will show how these data, without explicit knowledge of the individual frame orientations and with less than 100 photons per pattern, can be used to reconstruct a 3D diffraction volume in Fourier space using the Expansion-Maximization-Compression algorithm [3]. This diffraction volume is then used to reconstruct the real-space density of the particle by conventional iterative phase retrieval.

The influence of various levels of experimental background noise will be discussed.

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Three Dimensional *In Operando* Imaging of a Semiconductor Heterostructure through X-ray Bragg Ptychography

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ABSTRACT

For characterizing with nanoscale resolution the crystalline properties of a material, X-ray ptychography is a method complementary to electron microscopy techniques in that it allows to image *in operando* buried specimens up to several micrometres thick. Since its proof of principle published in 2011 [1], 3D Bragg ptychography results greatly improved in robustness, resolution and sensitivity [2,3]. Recently, we succeeded in imaging a nanostructured thin film extended in the two planar directions [4]. The experiments were performed at the nanofocused ID13-ESRF beamline. The sample was an InP/InGaAs multilayer bounded onto a Si wafer with a thin oxide layer, as desired for optimizing the optical index contrast. Some key steps in data acquisition and reconstruction algorithms are presented in this talk. These result in a 3D image with large field of view (2x0.4 µm²), nanoscale resolution (9 nm along the thin film thickness), strain and tilt sensitivity below 10^{-3} and 0.005° respectively.

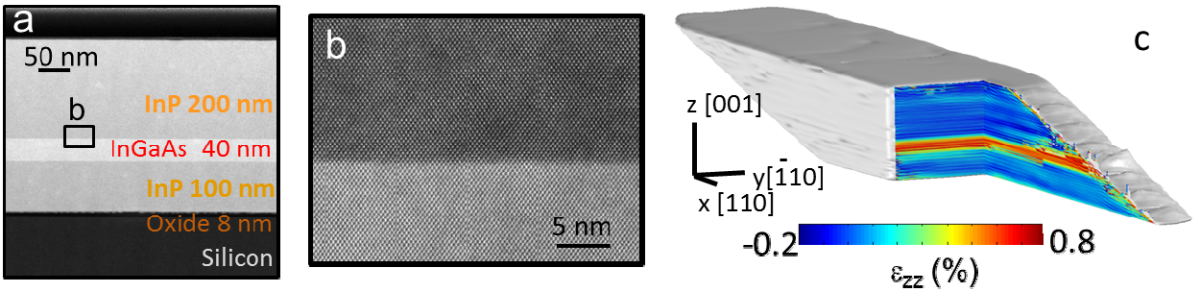

Figure 1: (a) Structure of the thin film on a scanning transmission electron microscopy image (high-angle annular dark field mode). (b) Zoom in on the top InP/InGaAs interface. (c) 3D Bragg ptychography strain result; the InGaAs layer is clearly evidenced, as well as some fluctuations inside the InP layers (the length of the black lines is 200 nm).

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Direct Single Shot Characterization of the Spatial Coherence of XUV and X-ray Sources

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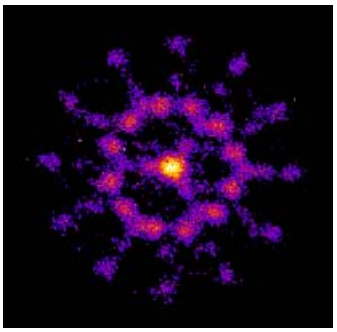
ABSTRACT

XUV sources generated by HHG or FEL provide pulses with a partial spatial coherence [1-2]. As the diffraction of the field depends on its coherence, a prior knowledge of the spatial coherence is needed for application where the diffraction is involved. This is the case in lensless imaging, where the quality of the image reconstruction is related to the degree of coherence of the illuminating light source [3, 4, 5]. The degradation of the image resolution is related to the use of the full coherence diffraction formalism when the illumination is only partially coherent. To overcome this effect, the measured spatial coherence of the source can be used as an input in the image reconstruction process. Furthermore, knowledge of the coherence of the source allows studying the physics of the generation [6, 2].

Up to now, all the methods to characterize the spatial coherence require the knowledge of the intensity distribution of the incoming field or the measurement of the field at different planes. A parallel characterization of the intensity requires XUV beamsplitters; however those are not readily available at those wavelengths. Moreover, there is a need for single shot characterization technique to avoid any error induced by shot to shot beam fluctuations.

Experimental diffraction pattern of a source at λ=24 nm through the 2D NRA.



We present here a new method to characterize the spatial coherence that fulfills those requirements. It is based on a variation of the spatial coherence characterization with multiple apertures [7] that allows measuring the spatial coherence at different vectors of separation $\mathbf{d}_{nm}$ with only one far field interferogram. Our method uses a multiple aperture interferogram generated by a 2D NRA (non-redundant array) of apertures, designed to generate a consistent set of solvable equations that allows calculating the spatial coherence and the intensity at the position of each aperture. The only required condition is that the magnitude of the spatial coherence is shift invariant, without any restriction on the phase of the spatial coherence. We will present experimental results using a HH source at a wavelength of 24 nm that validates the proposed method in single shot. We will raise issues about spatial coherence measurements in multiple shot acquisitions.

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Statistical Properties of the Free-electron Laser FLASH Measured by the Hanbury Brown and Twiss Interferometry

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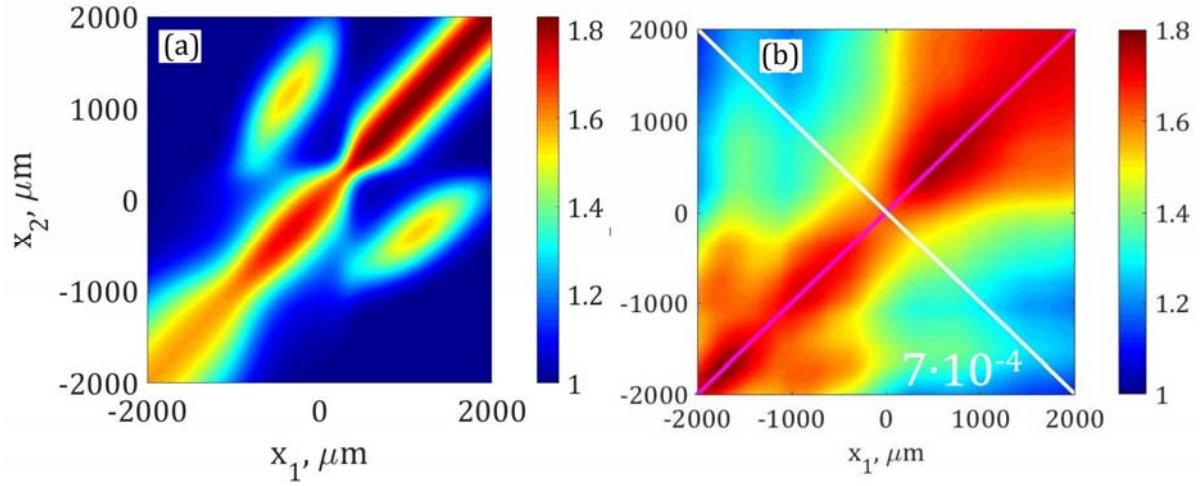
ABSTRACT

We present a comprehensive experimental analysis of statistical properties of the self-amplified spontaneous emission (SASE) free electron laser (FEL) FLASH by means of Hanbury Brown and Twiss interferometry. The experiments were performed at the FEL wavelengths 5.5 nm, 13.4 nm and 20.8 nm wavelengths. At all wavelengths and operating conditions of FLASH we obtained high degree of spatial coherence: approximately 0.7 for shorter wavelengths and approximately 0.5 for 20.8 nm. We observed an evidence of the presence of multiple secondary beams in the FLASH radiation. We have developed a model for the behavior of the multiple beams (Fig., (a)) and their effect on intensity-intensity correlation function, which allows us to describe the observed features (Fig., (b)).



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Coherent X-ray Scattering Beamline at Taiwan Photon Source

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ABSTRACT

The 3 GeV Taiwan Photon Source (TPS) with low emittance 1.6 nm-rad, which provides the extremely brilliant and highly coherent X-ray beam, is being commissioning at the National Synchrotron Radiation Research Centre, Taiwan. The coherent X-ray Scattering (CXS) beamline is one of the seven phase-I beamlines at TPS. This beamline equipped with two in-vacuum undulators provides coherent photon flux greater than 1010 photons per second at 6 keV X-rays. The X-ray beam is monochromated by a double crystal monochromator with energy resolution 2x10-4 by using Si(111) crystals. Kirkpatrick-Baez (KB) mirrors are used to focus the X-rays down to 1 μm2 in the energy range from 5.6 keV to 20 keV. The sample-to-detector distance can be varied with a range of 0.7-12 m. State-of-the-art detectors of Eiger X 16M and 1M are equipped for data collection of 133/750/3000 Hz frame rates with region-of-interest technique.

Combined the highly coherent X-rays and state-of-the-art detectors, the CXS beamline at TPS provides advanced lensless microscopy for millisecond and nanometer scales using coherent diffraction imaging (CDI) and Bragg CDI techniques. The CXS beamline will open to general users in 2016.

Figure 1: Drawing of coherent X-ray scattering beamline at TPS.

Tabletop Ultrastable Fourier Transform Interferometry at 17 nm Wavelength using High Harmonics

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ABSTRACT

High-Harmonic Generation (HHG) is a process that coherently generates broad bandwidth extreme ultraviolet (XUV) and soft-X-ray light, making it a promising source for interferometry and Fourier Transform Spectroscopy with short wavelength radiation. For this type of application a pulse pair with a controllable delay and a stable phase is required. Such a pulse pair can be obtained with a split-mirror as XUV beamsplitter [1,2], but it requires expensive high quality XUV optics. However, HHG can also produce phase-locked XUV pulses by driving the process with a pair of spatially separated, but identical near-infrared pulses.. For this purpose we developed a common-path interferometer based on four birefringent wedges, similar to the interferometer developed by Brida *et al.* [3]. Tilting the last wedge separates the two pulses spatially in the focus for HHG generation, but leads to overlapping XUV beams in the far field, as shown in Figure 1.

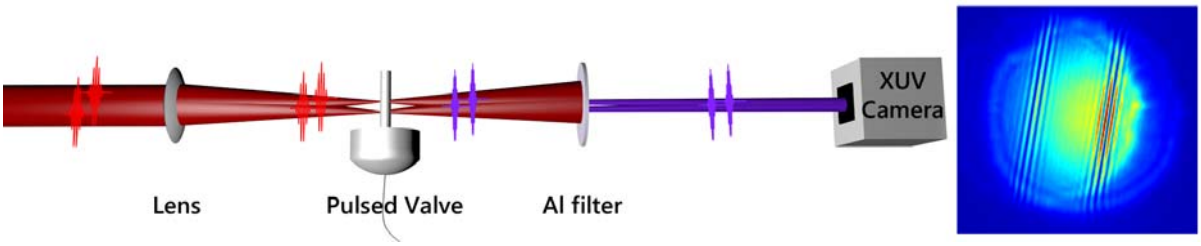

Figure 1: Schematic overview of the HHG setup. Two coherent infrared pulses produce HHG independently in a gas jet, and the resulting XUV pulse pair is detected with an XUV-sensitive CCD camera for interferometry and spectroscopy.

Pairs of 1 mJ, ~20 fs pulses are used to produce high harmonics in either argon, krypton or neon. By capturing the XUV interference on a CCD camera while scanning the delay, we reconstruct the full HHG spectrum by Fourier transformation. Wavelengths as short as 17 nm are detected when neon is used as the interaction medium. A major advantage of our approach is that we recover a spectrum for each pixel on the detector. With respect to coherent diffractive imaging applications, this allows us to resolve different diffraction patterns for the individual spectral components of the XUV radiation, enabling broadband XUV lensless imaging [4].

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Structural Information beyond the Powder Average from Colloidal Crystals using X-ray Cross-correlation Analysis

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ABSTRACT

Structural features of crystallites in solutions whose orientation cannot be controlled experimentally are usually studied by evaluating the angular mean of the X-ray scattering signal averaged over a large number of measurements from random particle configurations. Structural information beyond the angular mean can be obtained using angular cross correlations (XCCA) [1]. Here, we analyse the angular structure of colloidal nanocrystallites in a dilute colloidal sample system composed of a copolymer of butyl acrylate and trifluoroethylacrylate in aqueous solution. We compare the measured angular correlators with simulation data from small fcc, hcp and rhcp nanocrystals.

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Bragg Ptychography Imaging of Phase-ordering Fe-Al Alloys

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ABSTRACT

We performed coherent x-ray diffraction imaging (CXDI) in Bragg scattering geometry using the ptychography [1,2] setup at beamline ID01 of ESRF. In addition, ptychography in transmission geometry was employed on a standard sample (Siemens star) to yield an independent estimate on the illumination function and provide a general test of the setup. This experimental scheme has capability of imaging the phase shift of the sample which is related to the atomic structure. Fe-Al alloys display phases where the atoms order on sub-lattices resulting in the emergence of superlattice reflections that otherwise are forbidden in the bcc structure. The degeneracy of the ordered structures results in domain boundaries that, in addition to the general strain of the lattice, will give a phase shift depending on which superlattice reflection is probed. We investigated the B2 phase of $Fe_{60}Al_{40}$ and the D03 phase of $Fe_{72}Al_{28}$ specimens [3,4] with the aim of imaging the ordered domain structures and a detailed analysis is in progress.

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Ptychotomography at DLS Coherence Beamline I13

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ABSTRACT

Ptychography has emerged as an important technique for high resolution, high contrast imaging [1,2]. A natural extension of two dimensional ptychographic imaging is the three dimensional analog, ptychotomography. We exploit the high resolution 2D ptychographic projections obtained at various angles as a starting point which are then taken through the conventional tomographic process of alignment and 3D reconstruction thus obtaining a three-dimensional transmission map of the sample under study [3].

We will report about the demonstration and execution of ptychotomography at I13-1, the coherence branchline at Diamond Light Source [4]. We were successful in collecting the three dimensional ptychotomographic data from the nanoporous gold sample. The sample was imaged at an energy of 8.4 keV. The Merlin detector with a pixel size of 55 microns and 515x515 pixels wide was employed. Presented below are the 2D reconstructions at −90,0,90 degrees. The dataset is presently in the analysis stage. We are currently in the process of achieving faster scan rates and making further improvements to the existing 3D data acquisition and reconstruction routines. We are headed towards execution and optimization of multi-wavelength imaging and on-the-fly scanning ptychotomography.

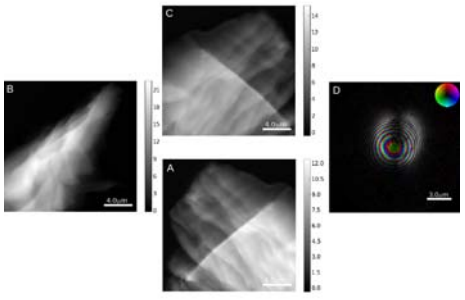

figure 1: A,B,C. shows the phase unwrapped projections of nanoporous gold sample at -90,0 and 90 degrees respectively. The gray scale shows the phase shift in radians. D is the first mode of orthogonalized probe obtained from reconstructions.

We acknowledge financial support through the European Research Council (ERC, starting grant “OptImaX”).

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X-ray Cross-correlation Approach in Nanoscale Structural Studies of Partially Ordered Systems

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ABSTRACT

Materials with complex or smart functionality are often associated with structural complexity, which can be achieved, for example, through sophisticated spatial arrangements of constituents, chemical diversity or intricate dynamics. Our understanding of material properties is largely determined by detailed knowledge of their nanoscale and atomic structure, and advances in materials research strongly rely on the availability of relevant characterization tools. The x-ray cross-correlation analysis (XCCA) is a coherence technique that can provide rich information covering a wide range of structural properties of non-crystalline systems, from local structure to medium range order [1-3].

We present our recent results of experimental studies based on the XCCA of the scattered intensities from different types of disordered and partially ordered systems. XCCA of the scattering data measured from liquid crystal films enabled high-precision quantitative studies of the bond-orientational order [4, 5]. Application of the nanoprobe x-ray beam with subsequent XCCA [Figure 1] also allowed us to construct spatially resolved maps of morphology and structural inhomogeneities in semicrystalline polymer blends [6, 7].

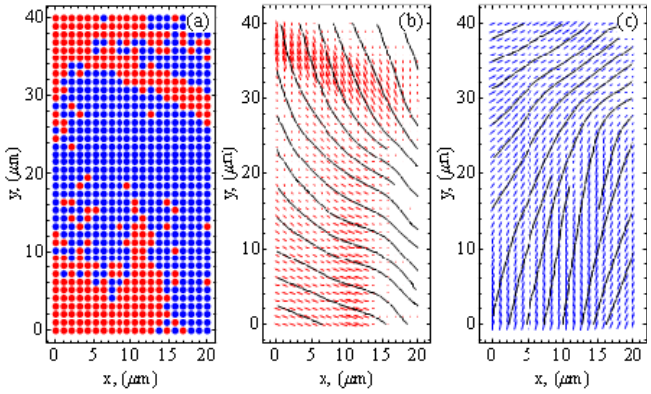

Figure 1: (a) Spatial distribution of distinct morphologies of crystalline poly(3-hexylthiophene) (P3HT) domains across the semicrystalline film, determined from the orientations of the (200) (b) and (020)/(002) (c) scattering peaks. Sample areas with predominant face-on (red points) and mixed (blue points) orientation of crystalline P3HT domains are visualized in (a).

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Evolution of Inversion Domain Boundaries along GaN Nanowires

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ABSTRACT

We report on the study of the displacement field induced by several Inversion Domain Boundaries (IDBs) in Gallium Nitride (GaN) nanowires with a spatial resolution better than 10 nm and a displacement accuracy of a few picometers. Recently, picoscale displacements along and across the wire were directly extracted from several Bragg reflections using phase retrieval algorithms, revealing rigid relative displacements of the domains and the absence of microscopic strain away from the IDBs [1]. This experimental displacement field differs from the one predicted by the theoretical work of Northurp et al. [2]. A possible explanation to the discrepancy between experimental and numerical results is the segregation of silicon atoms in the IDBs.

Today we would like to present new experimental results on samples grown with or without variations of silicon content. Several Bragg reflections have been measured at different heights of the wires. An evolution of the inner structure has been revealed; the IDBs configuration and the displacement field evolve both along the wire. The IDBs tend to be aligned on the (100) planes. More surprising, the ratio of Ga-terminated / N-terminated domain increase and the displacement field evolves of few picometers between the bottom and the top of the wire. Additionally, no effect of the variation of silicon content has been evidenced.

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Coherent X-ray Diffraction Imaging of Ferroelectrics Domains in Perovskite Thin Films

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ABSTRACT

Ferroelectric thin films demonstrate various domain structures, in the range of a few to a few hundred nanometres in size, depending on their composition, thickness and the substrate upon which they reside [1]. Extremely dense and highly inhomogeneous domain structures can be engineered in ultrathin films [2], which is especially interesting in the light of the recent discoveries of unusual functionalities at ferroelectric domain walls [3]. Coherent x-ray diffraction offers an insight into the structure of such materials in the form of ptychography [4].

Here, the ferroelectric domain structures of thin films (30-50nm) of PbTiO3 deposited via sputtering on both DyScO3 and KTaO3 substrates were investigated using a ptychographic approach. The preliminary results of our study will be presented.

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Transverse Coherence Properties and X-ray Photon Correlation Spectroscopy at SACLA

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ABSTRACT

With the rise of free-electron lasers (FEL) operating in the hard X-ray regime, physical and chemical processes can be studied on ultrafast time scales with molecular resolution. The superior degree of coherence of the FEL radiation allows, e.g., studies of sample dynamics by X-ray Photon Correlation Spectroscopy (XPCS) or single particle imaging with unprecedented accuracy and at ultrashort acquisition times below 100 fs. Due to the self-amplified spontaneous emission (SASE) process used to generate the FEL radiation, the beam position and intensity fluctuates on a shot-to-shot basis. Thus, the coherence properties of the radiation have to be studied for single shots in order to quantify the influence of such SASE fluctuations on the experiment.

First, we present studies of the coherence properties of the free-electron laser SACLA in the hard x-ray regime [1]. We performed a small-angle X-ray scattering (SAXS) experiment on colloidal particles giving rise to speckle patterns. The degree of coherence was extracted for single X-ray pulses by performing a contrast analysis on individual speckle patterns. On average, we found an almost full transverse coherent beam reflected by a speckle contrast of 0.79 with a shot-to-shot variation of 0.09 (standard deviation). These results will be compared to our recent findings from the LCLS [2,3].

Second, we discuss a proof-of-principle sequential XPCS study at SACLA [4]. By analyzing speckle patterns from static and diffusive colloidal sample systems we demonstrate the feasibility of XPCS at FEL sources for prototypical soft matter systems. We extract a contrast from the correlation function of 0.4 which is half of the value obtained from single shots [1]. These results are modeled by simulations of diffusive particles probed by X-ray pulses that vary on a shot-to-shot base with respect to coherence, pointing stability and beam size. Most importantly, we did not observe any effects from beam-induced heating due to the pulse structure of SACLA.

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X-ray Nano Coherent Scattering on GaP/Si for III-V Monolithic Integration on Silicon

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ABSTRACT

GaP, quasi-lattice matched to Si, allows growth of low defect density III-V/Si pseudo-substrates [1]. However, Antiphase boundaries (APB) likely appear and must be avoided. In this context, X-ray nanodiffraction and Bragg coherent diffraction imaging (BCDI) have been used as non-destructive techniques for local characterization of APB configuration [2]. Different GaP/Si nanolayers were studied at ID01/ESRF with an 8 keV coherent xray beam. Here a 140nm thick GaP presents annihilated APB (less than 3/μm emerging APB). Bragg geometry ptychography of the APB has been attempted using (002) GaP weak reflection. This shows a peak splitting, characteristic of a heterogeneous APB density. But a still too high defect density precludes successful phase retrieval imaging. Two-dimensional fast mapping (kmap) [3] over the (004) and the (002) reflections shows for different regions of integrated intensities (ROI) (Fig. 1a) weak (Bragg maximum -0.5° on rocking angle) and strong scattering conditions (Fig. 1b and 1c respectively). As shown fig. 1b), the weak scattered intensity in ROI1, exhibits contrast lines oriented along both [1 1 0] and [-1 1 0] crystallographic directions. This contrast corresponds to regions of high tilt, surrounding misfit dislocations [3]. Strong scattering conditions performed on the (004) (Fig. 1c) and the (002) Bragg reflections present a quite different contrast with large spotty regions. We believe that this anisotropic contrast is due to weak tilt/strain, associated to the APD annihilation process.

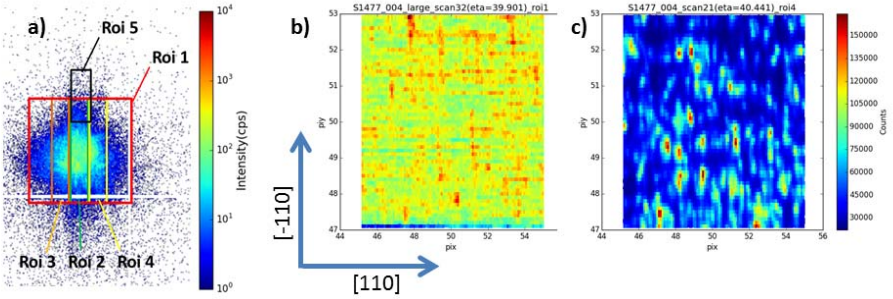

Fig. 1 a) ROI definition b) ROI1 weak beam (-0.5°) 10x6μm^2 kmap on GaP(004). c) ROI4 strong beam kmap on GaP(004).

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Flow-aligned Single-particle Diffractive Imaging of 3D-DNA Nanostructures in Liquid Jets

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ABSTRACT

X-ray free-electron lasers open up the possibility to determine molecular structures of macromolecules to viruses, by aggregating diffraction patterns recorded from uncrystallised particles with intense femtosecond-duration single X-ray pulses. A key challenge is to either constrain the orientation of the particle or to determine it from each of the very noisy diffraction patterns. This project addresses these challenges using DNA nanotechnology. A DNA “rigid tail” is attached to the macromolecule to flow-align it in a liquid jet, and also provides a strong holographic reference. The computational design and production of the DNA construct has been achieved, which was used to secure beamtime at LCLS to demonstrate the idea. In this poster, we present the recent experimental results obtained from LCLS.

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Pinhole-CDI: Unique and Deterministic Phase Retrieval via Beam-confinement

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ABSTRACT

Coherent Diffractive X-Ray Imaging (CDI) enables nanoscale imaging of samples in their natural state, but requires a phase retrieval step that suffers from non-convexity and latent non-uniqueness [1-3]. Holographic approaches overcome the latter drawbacks by observing the superposition of the unknown object signal with a known reference wave, typically generated by a sharp speckle located at some finite lateral distance to the object [4-6]. However, these benefits come at the cost of considerable modifications of the CDI-setup and increased exposure requirements.

Here, we argue that a beam-confining circular pinhole, as employed in conventional CDI-setups, already shapes a characteristic reference wave of considerable value. For a setting where the object is placed directly in the exit of the pinhole, we show absolute uniqueness of the phase reconstruction without trivial ambiguities. This analytical result is supported by numerical simulations [7] of the arising holographic phase retrieval problem as well as by an experimental proof of concept. We observe that iterative phase retrieval algorithms converge in a stable and deterministic manner for noisy intensity data, promising superior robustness of the proposed pinhole-holographic approach compared to conventional CDI.

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Progress Towards Dichroic Bragg Coherent Diffractive Imaging

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ABSTRACT

Synchrotron-based hard x-ray sources have enabled revolutionary breakthroughs for probing magnetism and strain at the nanoscale. However these advancements have mostly followed separate tracks, with magnetic techniques and strain techniques evolving independently. Many of these advanced methods to study magnetism[1] and strain[2] are performed in the Bragg-diffraction geometry, offering the possibility of combining them into a single probe carrying dual information.

We are developing dichroic Bragg Coherent Diffractive Imaging (BCDI) for simultaneous three-dimensional imaging of strain and magnetization at the nanoscale.[3] To enable dichroic BCDI experiments, we installed a diamond x-ray phase retarder at beamline 34-ID-C of the Advanced Photon Source. This setup delivers a 0.6 μm focused, circularly polarized, coherent x-ray beam to the sample. A pixel array detector mounted on the Kappa diffractometer arm at 34-ID-C, typically a Medipix 2 camera, records the coherent diffraction patterns. We describe the concepts behind dichroic BCDI then discuss our recent progress. This includes BCDI reconstructions of non-magnetic Au nanocrystals taken with the phase retarder as seen in Figure 1, showing it has minimal impact on the nanocrystal reconstruction quality. Additionally, we report dichroic diffraction experiments on a bulk magnetocaloric $Gd_5Si_2Ge_2$ crystal taken with the sub-micron coherent beam, and preliminary dichroic BCDI results obtained with magnetic PtCo nanocrystals.

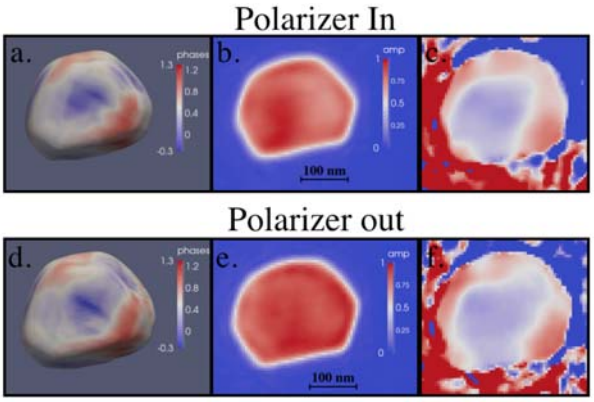

Figure 1: Top row: Gold nanocrystal reconstruction with the phase retarder in the beam showing (a) magnitude isosurface (25%) colored by phases (b) magnitude slice (c) phase slice. Bottom row: Reconstruction of same gold nanocrystal with the phase retarder out of the beam, showing (d) magnitude isosurface (25%) colored by phases (e) magnitude slice (f) phase slice.

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Towards Single-shot Measurements of Focused FEL Wavefronts using Iterative Phase Retrieval

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ABSTRACT

The advent of Free-Electron-Lasers (FELs) enables new insight into many fields of science. These new sources provide ultra short, high peak brilliance and coherent pulses, offering numerous scientific opportunities ranging from observing optical nonlinear effects, to study matter in extreme conditions, to explore dynamics of matter and imaging the structure of non-crystalline biological samples.

However, at currently operating FEL sources, the pulsed radiation produced primarily relies on the stochastic process of Self-Amplitude Spontaneous Emission (SASE), originating from random fluctuations in the driving electron bunches. Thus the complex wavefronts can fluctuate dramatically from shot-to-shot and posses stochastic features in every single shot.

Intuitively, a detailed understanding of FEL based experiments requires potentially prior knowledge of the spatial distribution of each complex wavefront[1]. We report on a high resolution coherent imaging technique, based on the modified near field phase retrieval algorithm[2], to fully characterize single-shot highly focused FEL pulses[3].

Exploiting the strong curvature of a divergent beam downstream of the focal plane, ensures the uniqueness of the iterative solution and reliable, fast convergence[4]. This method can be compared with Hartman Wave Front Sensing (HWS), a well-established, but relatively low-resolution method for characterizing long wavelength FEL beams[5]. We demonstrate that the new method exploits invaluable high resolution information, integrated into the wavefronts which cannot be understood utilizing HWS.

We show complex wavefront reconstructions for many individual pulses collected at a variety of different source parameters. The difference between individual pulses for the same source parameters, as well as the difference between sets of pulses for different source parameters are explored. This statistical overview can help to potentially connect the reconstructed wavefronts to the relevant ideal source parameters, as well as exploring the natural variations of FEL wavefronts for different source parameters.

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Phasing in Protein X-ray Crystallography using Data from Multiple Unit Cells

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ABSTRACT

Direct Methods have provided an *ab initio* phasing method for small molecule X-ray crystallography and are considered to have generally solved the phase problem for small molecules. The case is different for crystallography of larger molecules like proteins. Even though a majority of proteins can be solved by molecular replacement, this method cannot be applied to new folds and has the problem of model bias.

Here we propose an *ab initio* phasing method that doesn't need prior information about the protein structure. The basic concept is explained by Sayre (1952) (1) who pointed out that the Bragg diffraction under-samples Fourier space relative to the information needed for uniquely determining the phases. Diffraction data from a crystal of the same protein but with a different unit cell will sample different regions of Fourier space. Many protein crystals can be obtained in different unit cells – either by changing the crystallization conditions or by changing the solvent content (dehydration) – and therefore potentially provide the additional information needed. Already in 1952, Bragg and Perutz sought to get phase information from crystals with different solvent contents. (2)

We have tested the feasibility of this approach by running 3D simulations with two ideal protein crystals with different unit cells sizes. Using modern iterative projection algorithms we can successfully reconstruct the real space electron density from simulated Bragg diffraction data from the two unit cells. Our simulations assume that the protein structures are identical in the two unit cells, and that their envelopes, and their positions and orientations in the unit cell, are known. We are currently investigating how these parameters can be determined as part of the phasing process.

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Phasing XFEL Diffraction Data from very Small Crystals

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ABSTRACT

One of the key advantages of XFELs is that diffraction data can be recorded from crystals smaller than those that can provide usable data from synchrotron sources. In many cases, these small crystals can be much easier to produce than macroscopic crystals. An additional advantage of using very small crystals is that they may provide measurable diffraction between the Bragg peaks. As was first pointed out by Sayre [1], measurement of this data provides a possible direct route to solving the phase problem. Although the problem in this form is rather easy to state, in the context of serial femtosecond nanocrystallography (SFX) there are a number of hurdles that need to be overcome for practical implementation. First, it has been shown that diffraction between the Bragg peaks for a small crystal in a nontrivial space group depends on the nature of the edge termination of the crystal. Different edge terminations can be modeled by considering the crystal to be made of different, related, unit cells [2,3,4]. Since SFX diffraction data are averaged over many crystals, the diffraction is averaged over many crystal edge terminations or unit cells. Interpretation of the data then requires a model of the kinds of unit cell present. Second, extraction of the molecular transform intensity from the crystal data is noise sensitive. Third, reconstruction algorithms are needed that take into account the presence of crystals with multiple kinds of unit cell. Progress has been made on addressing these problems and successful reconstructions of simple fabricated structures from soft x-ray data from individual two-dimensional crystals have been reported [5]. Application to protein nanocrystals is more challenging. Diffraction by nanocrystals will be reviewed and alternative reconstruction algorithms for data derived from clusters of molecules forming different unit cells will be described. Finally, possible models of Cathepsin B [6] nanocrystals will be considered and used to simulate the inter-Bragg diffraction, which is compared with the SFX data.

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CATERETÊ: The Coherent and Time-resolved X-ray Scattering Beamline at the Brazilian Light Source SIRIUS

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ABSTRACT

The Cateretê beamline at SIRIUS synchrotron source will be dedicated to coherent and time-resolved scattering experiments. It will provide unique capabilities in biological and soft materials imaging and dynamics experiments with particular focus on the application of coherent X-ray scattering. Coherent X-ray diffractive imaging (CXDI) and X-ray photon correlation spectroscopy (XPCS) experiments will be at the heart of the activities planned at the Cateretê beamline. The beamline will enable to image biological specimens such as parasite cells, yeast spores, chromosomes and viruses but will also extend the imaging possibilities to larger biological specimens, up to 30 μm² with unprecedented resolution of 10 nm. The high coherent hard-X-ray flux of Cateretê will enable to perform *in situ* 3D CXDI experiments with a particular focus on operando measurements for catalysis.

The SIRIUS storage ring is designed to have a horizontal emittance of ε_x = 246 pm.rad and a vertical emittance of ε_y = 2.46 pm.rad. The Cateretê beamline will be located on a low β straight section and equipped with an in-vacuum undulator (IVU) of 19 mm period and 2 m length.

The Cateretê design and the latest wave-propagation simulations of the partially coherent beam will be presented. Cateretê aims to offer the largest coherent X-ray beam at the sample position, ~0.05 x 0.05 mm², as well as very intense coherent flux, > 10^{10} ph/s. The beamline will be operating in the 3 to 20 keV energy range using a large in-vacuum Medipix pixel detector (55 x 55 μm²) for imaging biological and nanomaterials. The sample-to-detector distance will be remotely controlled and variable from 50 cm up to 8 m, enabling to carry out ultra-SAXS in the pinhole geometry, q_{min} ~ $1 \cdot 10^{-4}$ Å^{-1}. Finally yet importantly, pink beam operation is envisaged for time-resolved experiment requiring extremely large flux.

Soft X-ray Resonant Magnetic Scattering on Artificial Spin Ice using a Coherent High Harmonic Beam

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ABSTRACT

We study artificial square ice, which is a metamaterial produced by electron beam lithography[1], and consists of dipolar-coupled nanomagnets placed at the sites of a square lattice (see Figure 1a). These permalloy (20% Fe, 80% Ni) nanomagnets with a few tens of nanometers dimensions are small enough to ensure single-domain magnetic behavior and their volume can be varied to modulate their stability at room-temperature. The interaction between the nanomagnets induces a spin ordering that can be studied with soft x-ray magnetic scattering (SXRMS) [2]. Here, we use the soft x-ray high harmonic radiation from a table-top laser, which has the advantage of femtosecond time resolution and easy access. We study magnetization dynamics of artificial spin ice around the M-edge absorption of Fe and Ni. For a square lattice with ground state magnetic ordering [2]–[4] simulations based on kinematical theory of x-ray scattering [5] predict the appearance of additional magnetic Bragg peaks in the diffraction pattern, as shown in Ref. [2] (see Figure 1b). In this contribution we will describe our approach to study artificial spin ice with a high harmonic generation beamline and show our most recent results.

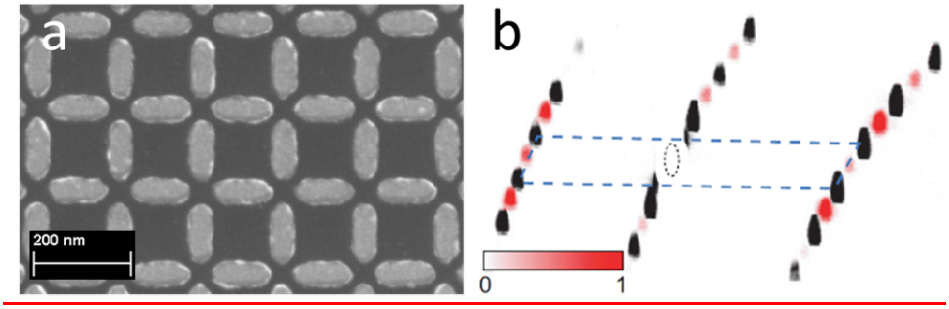

Figure 1 : a) Spin ice sample b) Experimental scattering pattern of Artificial Square Ice recorded at the Fe L_3 edge (706.8 eV). The Bragg peaks highlighted in red are of pure magnetic origin and the black peaks are of combined structural/magnetic origin. Taken from [2]

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Probing Nanosecond Dynamics at LCLS using the Hard X-ray Delay Line

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ABSTRACT

We report on a successful implementation of the hard X-ray delayline [1,2] at the Linac Coherent Light Source. The device is capable of providing two X-ray pulses with controllable time delays ranging from a few femtoseconds to nanoseconds, which is sufficient for probing ultrafast phenomena in versatile choices of condensed matter systems. The measured throughput of the device within 1.47e-5 energy bandwidth of the exit beam at 7.9 keV is 30% [3]. The X-ray FEL pulses after the X-ray delayline are used to generate high (69%) contrast speckle patterns from nanoparticles, which is only possible due to the well preserved transverse coherence. Measuring intensity fluctuations also reveals that only a single or double temporal modes remain in the beam, indicating the delivery of near Fourier transform limited pulses.

We will also report on the results of a first proof of principle Split Pulse XPCS experiment.

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Characterization of Wavefronts at XFELS

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ABSTRACT

XFELs can achieve extremely high power densities within very small focal spots: this makes them suited for the study of weakly-scattering samples but at the same time highly sensitive to optics-induced aberrations. Because of this an in-depth knowledge of the beam's wavefront is very beneficial as it allows to find a plane in which such aberrations are minimized thus increasing the achievable resolution. Characterizing the wavefront is particularly interesting in the case of coherent diffraction imaging (CDI) experiments at XFELs where the properties of the wavefront can influence the performance of the reconstruction algorithms involved. In fact knowing the wavefront of an XFEL beam for a given experimental setup bears the potential to increase the achievable resolution. Up to now, only limited means have been made available to obtain an extended characterization of XFEL-generated wavefronts and the most advanced among them return information in either an averaged or a partial form [1-5]. Using ptychography, we are exploring ways to characterize individual wavefronts [6] and more precisely those of randomly stimulated self-amplified spontaneous emission (SASE) pulses. The strength of ptychography lies in the fact that it allows for simultaneous reconstruction of both the object's transmission function and the probe representing the complex-valued wavefunction interacting with it. During a ptychographic scan at XFELs it is usually necessary to average over many pulses and collect several diffraction patterns per scan position. This means that at first only an averaged probe is retrieved. Using multimodal decomposition such probe can be represented as the sum of different coherent modes each contributing to a different extent to form the individual diffraction patterns [7]. Further analysis can then reveal how much each of these modes contributes to each pulse thus effectively achieving pulse-to-pulse characterization, giving an unprecedented insight into wavefront fluctuations and advancing the development of online diagnostic techniques for XFEL beams and high-brilliance coherent beamlines in general.

We present preliminary results obtained from data collected at the LCLS.

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Development of a Lensless Microscope

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ABSTRACT

Lensless imaging is a promising technique that can take many forms in terms of experimental configurations: high harmonic generation, laser diodes,… In any case, the principle remains the same: a coherent beam illuminates a sample, forming a subsequent diffraction pattern on the other side, which is detected with a CCD camera. Since the phase information is intrinsically lost during the detection, one has to apply iterative algorithms in order to retrieve the phase and apply, either a Fourier Transform (in the far field regime), either the Fresnel propagator (in the near field regime).

In the CEA – Saclay, lensless imaging has been performed on the LUCA beamline (Laser Ultra Court Accordable). X rays are generated through high harmonic generation under vacuum via the interaction between a Ti:Sa laser beam (800nm) and a gas jet (argon or neon). Various reconstruction techniques have been used: Coherent Diffractive Imaging (CDI), Fourier Transform Holography (FTH) using circular references to encode the phase in the diffraction pattern [1], HERALDO (rectangular references)…

We propose a new design for lensless imaging, using a laser diode (400nm) and a CCD camera in the ambient air, forming a compact experimental setup with high performances. Although the wavelength is increased, one gains a lot in terms of space, number of photons, easiness of alignment and optimization, and signal to noise ratio.

Different configurations have been tested. More specifically, binary 2D objects, with a typical size of a few tens of µm, detected in the far field, reconstructed with existing phase retrieval algorithms, present a resolution down to the wavelength. We also performed 3D imaging: a pupil serves as a support for the field reconstruction, that can subsequently be back-propagated towards the sample placed close by [2].

On the other hand, if we want to look at bigger object, it is possible to perform in-line holography. For that, only the divergent beam is used, directly at the fiber output. The field of view can be extended to a few mm and go down to a few hundred of microns, with a resolution of a few microns. The twin image is eliminated via an iterative algorithm inspired by [3]. With this technique, amplitude and phase can be retrieved, thus it is possible to perform phase contrast microscopy.

This prototype paves the way to turnkey lensless diffractive imaging systems and presents large possibilities of applications (biology, surface analysis, …). We will present the prototype and the associated experimental results.

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Structure and Dynamics in Suspensions of Interacting Colloids Studied by Intensity Correlation Methods

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ABSTRACT

Intensity correlations methods in coherent X-ray scattering are particularly suited to study structure and dynamics of soft matter systems. Here, we present the results of an experiment performed on charge stabilized colloids (polyacrylate spheres dispersed in water).

Colloidal dispersions have been excellent model systems which have provided useful insights into the phase behavior of liquids and glasses [1]. The phase transition from ordered to disordered states can be induced for example by changing the particles concentration. Furthermore, for soft colloids the interparticle interaction potential can be varied from repulsive to attractive, by changing e.g. the solvent properties (such as salt concentration [2]). Hence, the phase diagram becomes more complex than for hard sphere systems.

In the present study we will discuss the influence of particle concentration and interaction potential on structural and dynamical properties of polyacrylate particle suspensions. The sample structure has been studied not only by conventional methods to obtain the static structure factor but also by the X-ray Cross Correlation Analysis (XCCA) technique which allows to access the samples local orientational order [3-6]. The structure factors at different particle and salt concentrations show the expected behavior with respect to peak height and position. In contrast the higher-order correlation analysis reveals an increase in the degree of the orientational local order for systems with higher salt content and with decreasing particle concentration. These structural observations will be connected with the samples dynamics which has been probed via X-ray Photon Correlation Spectroscopy (XPCS) [7].

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Efficient use of Coherent X-rays in Ptychography

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ABSTRACT

Ptychography[1] is a method of coherent diffraction imaging that applies translational diversity, in which the object of interest is scanned in small steps by an overlapping probe, providing redundancy in collected data. X-ray ptychography techniques rely on the realization of a fully coherent beam with high spectral purity. The efficient use of coherent X-rays is a crucial issue for the employment of X-ray techniques in synchrotron experiments. Recently, the mixed-state reconstruction algorithm [2] has been developed, in which blurry diffraction data are described as the sum of the diffraction intensities over multiple mutually incoherent illumination modes. Here we propose a means of efficiently using coherent X-rays in ptychography using the mixed-state reconstruction algorithm [3].

Our numerical simulation showed that a nearly diffraction-limited focusing X-ray beam can be described as an incoherent sum of a few orthogonal modes and that the first-mode flux significantly increases by relaxing the requirement on the degree of coherence. We performed its demonstration experiment at SPring-8. An increase in the first-mode dose improved the spatial resolution of the reconstructed image of a test object as shown in Fig. 1. The present approach enables the high-resolution and high-throughput observation of weak-phase objects in materials science and biology.

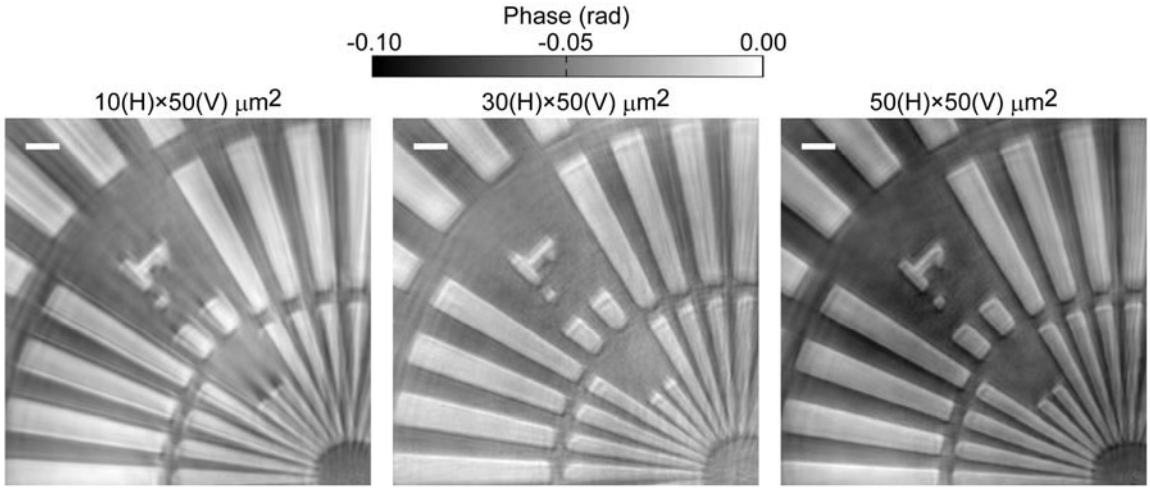

Figure 1: Phase images for the three slit openings reconstructed using the multiple-mode ePIE algorithm. The scale bar is 200 nm.

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Enhancement of Charge Ordering by Dynamic Electron-phonon Interaction. A Pump-probe Study at LCLS

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ABSTRACT

Symmetry breaking and the emergence of order is one of the most fascinating phenomena in condensed matter physics. It leads to a plethora of intriguing ground states found in antiferromagnets, Mott insulators, superconductors, and density-wave systems. Exploiting states of matter far from equilibrium can provide even more striking routes to symmetry-lowered, ordered states.

The advent of x-ray free-electron lasers opened up new routes to study structural dynamics on femtosecond time sales. Here, by utilizing the unique capabilities of the LCLS we demonstrate that moderate photo-excitation in elemental chromium can transiently enhance the charge-density-wave (CDW) order by up to 30% above its equilibrium value, while strong excitation leads to an oscillating, large-amplitude CDW state that persists above the equilibrium transition temperature. Both effects result from dynamic electron-phonon interaction, which provides an efficient mechanism to selectively transform a broad excitation of the electronic order into a well defined, long-lived coherent lattice vibration. This mechanism may be exploited to transiently enhance the order parameter in other systems with coupled electronic and lattice orders.

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Monodisperse Polymer Spheres for Benchmark Testing of Coherent X-ray Diffraction Imaging Techniques

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ABSTRACT

Coherent X-ray Diffraction Imaging (CXDI) has emerged as a valuable tool in a wide variety of scientific fields [1-5], enabling phase contrast imaging with 3D spatial resolution approaching 10 nm [6, 7]. Several CXDI-techniques exist, including “conventional” CXDI and ptychography. Common for most of these techniques is that they rely on iterative numerical reconstruction algorithms to retrieve real space images. Interpreting the reconstructed images can be challenging, as it requires experience to distinguish artifacts created by the reconstruction algorithm from real features. In addition the various CXDI techniques all have their own weaknesses and strengths. Conventional CXDI requires a known support, making it challenging to have complex sample environments, and twin-image problems are known to occur. The resolution acquired is however generally high. Ptychography, on the other hand does not require a support and imaging samples larger than 10 µm in complex *in situ* setups, are possible [2, 3], but the mechanical stability has to be accounted for to achieve the highest possible resolution. Standard absorption-based tomography can also be used for complex *in situ* studies and does generally not suffer from the same instability issues as ptychography, but it does not currently reach the same resolution as CXDI-techniques.

Here we present a comparison between different 2D and 3D imaging techniques utilizing phase shift and/or absorption as contrast mechanism. The experiments were performed at the ID10 beamline at the ESRF, and at the cSAXS (X12SA) and TOMCAT (X02DA) beamlines at the Swiss Light Source, Paul Scherrer Institute, Switzerland. Using monodisperse metal-coated polymer spheres (Ugelstad spheres) as test specimen, a comparison is made between conventional CXDI [8], ptychography [9] and standard radiography. By utilizing the fact that the polymer test samples are essentially identical, quantitative comparisons between the retrieved sample roughness, density, resolution, beam dose and reconstruction artefacts across several length scales can be made.

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Combined Ptychography and X-ray Fluorescence of First-row Transition Metals

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ABSTRACT

The low-emittance third-generation storage rings along with advances in instrumentation have established ptychographic coherent diffractive imaging in microscopic studies of nanoscale objects. Ptychography [1], a lensless imaging technique, offers quantitative measurements of optical density of even weakly phase-shifting samples at resolution beyond that of X-ray optics. Thanks to its scanning nature, ptychography can be directly combined with nanoscale X-ray fluorescence microscopy [2,3] which offers unique elemental contrast. Consolidation of these two techniques yields thus simultaneously complementary information on morphology and elemental distribution of investigated specimen facilitating further correlative study. Moreover, as ptychography is also capable of retrieving the illuminating probe [4], the resolution of X-ray fluorescence maps can be enhanced using 2D deconvolution.

We present the first implementation of simultaneous ptychography and nanoscale X-ray fluorescence microscopy at beamline P11 at the PETRA III synchrotron light source, DESY, Germany. An off-axis illuminated Fresnel zone plate was used to form a spatially coherent illumination [5]. Increasing the photon energy to 8.5 keV allowed us to obtain XRF signal from first-row transition metals. We will present ptychographic reconstructions with corresponding XRF maps of a dual-tone test structure. Spatial resolution of reconstructed images and deconvolved X-ray fluorescence maps will be evaluated using several resolution-estimation methods. Finally, challenges in multimodal imaging of weakly phase-shifting biological samples will be addressed.

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Sub-20 nm Resolution Coherent Diffractive Imaging with a Table-top XUV Source

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ABSTRACT

Coherent diffractive imaging (CDI) allows for lensless microscopy of samples illuminated with coherent XUV or X-ray light. It relies on reconstruction algorithms to retrieve the phase information from the measured intensity distribution of the diffraction pattern of the sample to obtain spatial information about the object [1]. Recently developed table-top fiber laser based XUV sources using high-order harmonic generation (HHG) from a gas jet offer unique opportunities previously accessible only at large scale facilities [2]. Here we present CDI experiments performed with a 68.6 eV XUV source, driven by a high-average power femtosecond fiber laser system. This source provides a narrow relative bandwidth ($E/\Delta E=200$), a good beam quality and a record-high photon flux. Refocusing of the XUV radiation by means of two concave dielectric XUV mirrors results in $4\cdot10^9$ photons/sec within a <10 µm diameter focal spot at the sample. In a first step, we analyzed the spatial coherence of the refocused beam. Diffraction from a double slit with 1.5µm separation shows an excellent contrast (>0.9) indicating a high degree of spatial coherence (see Fig. (1a)), which has been achieved by optimization of the XUV source. In a second step, we performed CDI experiments in a high numerical aperture configuration (NA=0.7). Figure (1b) displays a diffraction pattern which has been recorded with a shaped aperture object. It extends up to the edge of our detector with a good fringe contrast and a high signal-to-noise ratio. Thus, we expect a half-pitch resolution close to the Abbe limit of 13nm. A first reconstruction shown as inset in Fig. (1b) indicates sub-20 nm resolution, which is expected to improve to sub-wavelength with adequate curvature correction of the diffraction pattern [3]. Future scaling towards few-nanometer resolution table-top imaging is discussed.

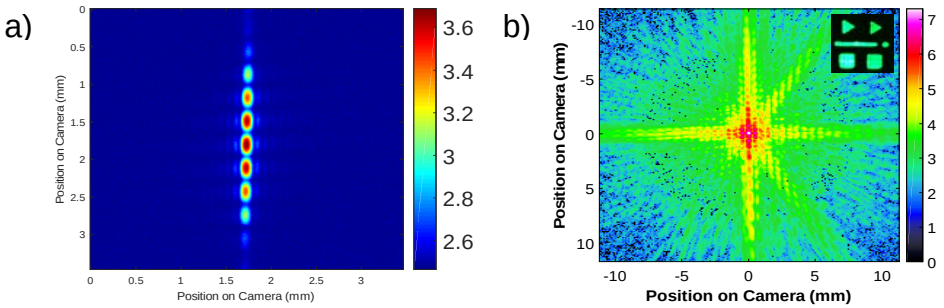

Fig. 1. (a) Diffraction from a double slit (1.5µm separation) shows excellent contrast (log-scale). (b) Diffraction pattern from a sample with 1µm dimension (NA=0.7). Inset shows a successful reconstruction of the object (log-scale).

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Single View Phase Retrieval of Extended Samples by Exploiting Sparsity

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ABSTRACT

Compressive sensing [1] is a signal processing technique which exploits sparse representations of the original signal to simplify processing operations. These ideas applied to synchrotron nanoscale imaging using phase retrieval is currently of great interest [2 – 5]. It exploits sparsity under some mathematical transformation of the quantity we wish to recover: rather than recovering the original non-sparse quantity, we apply a sparsifying transformation which "compresses" information into as few image pixels as possible, and then proceed to recover this simplified representation. We will formulate a non-convex optimization problem in this simplified sparse representation and derive an efficient Alternating Direction Method of Multipliers (ADMM) phase retrieval algorithm to solve this problem. Our ADMM method will be benchmarked on simulated samples of varying sparsity levels (ratio of the number of non-zeros to total problem size). We will then discuss sparsifying transformations when noise appreciably degrades measurements, which is one of the primary challenges when using compressive sensing ideas in phase retrieval. The use of compressive sensing ideas in phase retrieval offers the opportunity of imaging extended samples from a single view, a situation which usually requires ptychography. We also discuss ideas on how to improve upon existing ptychographic methods by incorporating sparsity exploitation into these methods.

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Domain Structure Retrieval of a Simulated Ferroelectric Film via 3D Bragg Ptychography

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ABSTRACT

In this work, we performed a numerical simulation of a three dimensional structural microscopy study on a nanostructured sample by 3D x-ray Bragg ptychography[1]. The specimen was modeled following a real perovskite ferroelectric thin film[2]: the lattice mismatch between the film and the underlying substrate is accommodated through a strain relaxation resulting in two crystallographic variants of the ferroelectric film material. There are organized as a quasi-regular domain texture.

In our model we considered a distribution of prismatic domains, with average planar size of 0.1 µm and thickness of 30 nm, illuminated by a beam produced by a Fresnel Zone Plate focusing optics, with spot size of about 2 by 0.75 µm. We calculated the set of 3D Bragg ptychographic diffraction patterns in the vicinity of the (001) Bragg reflection of the tetragonal domain, taking into account the photon shot noise.

Due to the complexity of the signal containing the contribution of a large number of domains together with the limited signal to noise ratio, we found that the inversion scheme had to be optimized. Different inversion strategies were tested, including different types of algorithms (preconditioned conjugate gradient and ordered-subset/PIE strategies[3] and different initial guesses (statistically equivalent or quasi-equivalent to the true numerical specimen).

The aim of this work is to optimize the acquisition, the analysis and the interpretation of the data acquired during the real experimental campaign. The advantage of pursuing this numerical experiment is that a complete *a priori* knowledge of the object to be retrieved, allows us to identify directly the critical issues related to the inversion procedure. Thereby, we assessed the dependence of the reconstruction quality with respect to the initial guesses, our main objective being to understand the amount of prior knowledge needed in the initial guess to retrieve successfully the true object. The simulation of the experiment is also a useful benchmark to test the capability of the ptychographic modality in retrieving a large and random collection of scattering objects with dimensions much smaller than the probe size.

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Bragg Coherent Diffractive Imaging of Defect Dynamics in Nanostructured Materials

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ABSTRACT

Nanostructured materials are essential to solving grand challenges in energy storage, environmental sustainability, and global climate stability given their novel properties relative to their bulk counterparts, including size-tunable thermodynamics[1–3]. “Defect engineering”, or the rational design and optimization of desired functionalities through deliberate defect manipulation, can be used to further optimize nanomaterial properties[4–7], but is limited in scope due to an inability of current probes to characterize defect dynamics under *operando* conditions in three-dimensional (3D) detail. Here I will discuss how Bragg coherent diffractive imaging (BCDI) can reveal the 3D dislocation distribution in single operating battery cathode nanoparticles[8], in palladium nanoparticles during the hydriding phase transformation, and in silver nanoparticles during dissolution. Our results point to interesting physics in single nanoparticles.

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Hanbury Brown–Twiss Interferometry at XUV Free-electron Lasers

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ABSTRACT

Measurements of second- and higher-order intensity correlation functions (so-called Hanbury Brown—Twiss (HBT) experiment[1,2]) performed at different XUV free-electron lasers (FEL) will be presented. First, we will present results of measurements[3,4] performed at SASE FEL FLASH at different wavelengths of 5.5 nm, 13.4 nm and 20.8 nm and at different operational conditions of the FEL. We demonstrate the high transverse coherence properties of the FEL beam with a degree of transverse coherence of about 80% and degeneracy parameter of the order 10^9 that makes it similar to laser sources. Intensity correlation measurements in spatial and frequency domain gave an estimate of the FEL average pulse duration of 30 fs. Our measurements of the higher-order correlation functions indicate that FEL radiation obeys Gaussian statistics, which is characteristic to chaotic sources.

Next, we will present results of measurements[5] performed at the seeded FEL FERMI. Our results indicate that this seeded source has, according to its 2-nd order statistics, rather a laser behavior.

In the end, comparison with the HBT measurements[6] at 3-rd generation synchrotron source PETRA III will be given.

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A New Approach for Phase Contrast Tomography under Conditions of Low Partial Coherence

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ABSTRACT

Hard x-ray tomography offers a unique capability to nondestructively map out the three-dimensional (3D) structure of a body or material. A major challenge for high resolution and/or phase contrast tomography is the requirement of high coherence radiation sources, impeding applications to be carried out with readily available laboratory sources, which typically exhibit only very low spatial coherence. By suitable generalization of the tomographic measurement geometry, one can relax the brilliance/coherence condition in one of the two source dimensions [1], opening up new opportunities to achieve nanoscale resolution with low brilliance sources such as laboratory x-ray tubes. To this end, we replace the two-dimensional Radon transform (2DRT), which is the common basis for most analytical x-ray tomography applications, with the three-dimensional Radon transform (3DRT). The area integrals required for the 3DRT can be realized experimentally, at least within geometric approximations suitable for analytical tomography, by a subsequent numerical projection of the acquired x-ray projection images. Two angular degrees of freedom enable the measurement geometry to cope with anisotropic beam properties.
We show the applicability of this 3DRT-based tomography scheme with experimental data and propagation-based phase-contrast tomography at anisotropic laboratory x-ray sources.

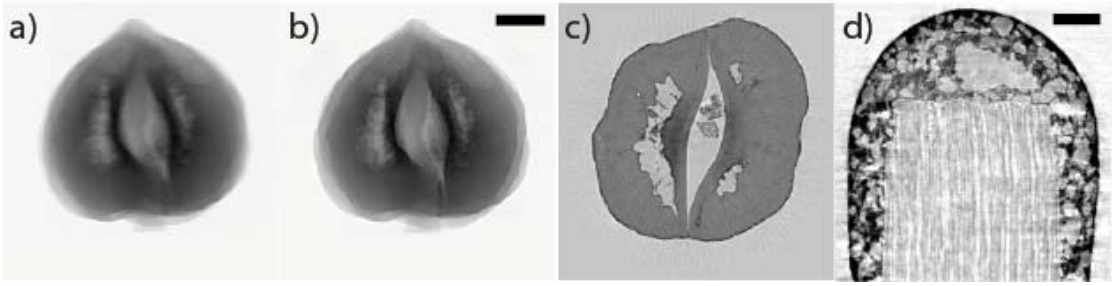

Figure 1: a) Acquired x-ray projection with an x-ray source spot of 1 x 0.1 mm (*horiz.* x *vert.*). The projection shows blurred side walls of the nut, while the top and bottom is sharply resolved. The reprojection (b) of the 3DRT-reconstructed nut shows high isotropic resolution. c) slice through the 3DRT-reconstructed nut. d) slice through a 3DRT-reconstructed match with Bronnikov-aided correction phase retrieval [2]. Scale bars: a)-c) 3 mm, d) 0.5 mm.

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Tomographic Coherent X-ray Diffraction Imaging of Bone and Dentin Ultrastructure

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ABSTRACT

At the nanoscale, bone tissue can be viewed as a composite material made of two principal components: collagen fibrils of ~ 100 nm in diameter and platelet-shaped calcium phosphate mineral nanocrystals of ~ 5 x 50 x 100 nm dimensions. The nanoparticles organization and structure in bone as well are of high interest by biomedical community since they have been identified as potential markers of bone quality and diverse pathological conditions [1].

Modern third-generation synchrotron radiation sources that are able to produce high-flux spatially coherent X-ray beams have opened new possibilities to develop various 3D X-ray imaging techniques for biological samples. One of such methods, CXDI is based on measuring the oversampled Fraunhofer speckle pattern of an isolated object and subsequent application of a phase-retrieval algorithm for image reconstruction [2].

The 3D CXDI reconstructions (ID10, ESRF) of human dentin and bovine bone samples of 5 µm3 geometry prepared by 3 different techniques (focused-ion beam and UV-laser microdissection of the ultramicrotomy slices and grinding), with a voxel size of 28 nm for dentin and 31 nm for bone respectively, will be presented. 3D nanoporosity in dentin and bone tissue is visualized, which existence has been postulated but not fully characterized by the biophysical community. Variations of mineral density were also observed in the hundreds nanometer range, which is to be compared with collagen microfibril diameter, implying mineral density changes at the fibrillar scale. The spatial resolution achieved by CXDI allowed not only to see internal ultrastructure of bone/dentin but also to visualize collagen banding pattern at the single fibril level. One can observe weak 1st order collagen peak in the diffraction patterns as well as repeated “dotty” pattern with the periodicity of 67 nm at the reconstruction.

However, current possible resolution, obtained by CXDI, is still not enough to visualize individual mineral crystals in bone which is the main goal of our project. Nevertheless, current results provide valuable insight in the ultrastructure of bone. Improving the spatial resolution down to 5 nm or less by solving current limitations is an ideal goal and could allow to conduct the first direct x-ray visualization of mineral crystals, studding their orientation and organization in strongly heterogeneous hierarchical bone tissue.

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Summed Image XPCS – A new Tool to Study Atomic Dynamics in Radiation Sensitive Samples

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ABSTRACT

XPCS has recently moved towards measuring atomic-scale dynamics in disordered and glassy samples [1,2]. In those experiments long series of thousands of speckle patterns are collected and analyzed in terms of intensity autocorrelation functions. This in turn implies that during a typical XPCS scan rather large total doses of 10^9 up to 10^{13} Gy are absorbed leading to beam damage even in hard condensed matter samples. This is much more severe for soft matter or biological samples excluding basically the measurement of atomic-scale XPCS up to now. Here we present a new XPCS method which allows us to reduce the absorbed total dose by orders of magnitude. The method enables us to measure atomic scale dynamics in radiation sensitive ionic liquids close to the glass transition and paves the way for XPCS experiments of the general class of soft and biological matter. The newly developed SIX technique (Summed-Image-XPCS) consists in taking two short exposures at the same spot and then quantifying the correlation between the two images as a function of the delay time t between the images. Every double-exposure is performed on a new spot on the sample spreading the absorbed dose over a large sample area. The degree of correlation between two images is equivalent to the intensity autocorrelation [3] and thus easy to analyze – in contrast to the integral approach of speckle visibility. We tested our concept on supercooled ionic liquids. Taking sparse double exposure speckle patterns we demonstrate the first successful measurement of atomic-scale dynamics in a radiation sensitive sample.

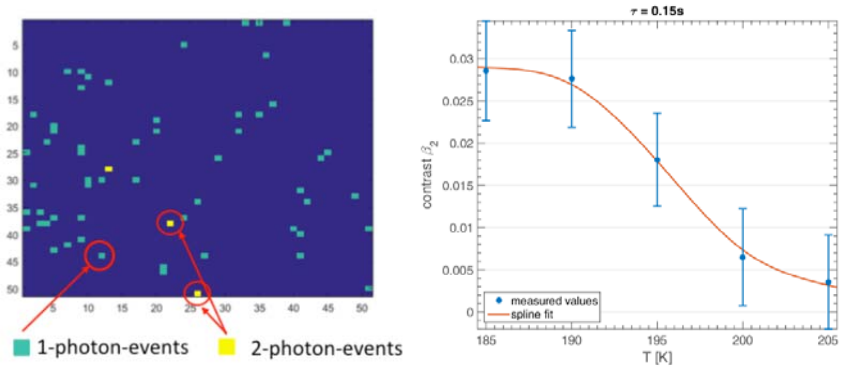

Fig 1: (left) Typical sparse speckle pattern with 1- and 2-photon-events. (right) Correlation function for a fixed time delay at different temperatures on the liquid structure factor.

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Imaging Criterion for Free-propagation Imaging Techniques at Free-electron Lasers and Synchrotrons

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ABSTRACT

The resolution of conventional coherent X-ray microscopy techniques at synchrotrons is limited by the radiation damage, and was claimed to be 10 nm for biological material [1]. Free-electron lasers (FEL) overcome this limit providing ultraintense and ultrashort pulses which overrun the damage formation[2]. Thus the resolution is limited by the number of photons available in a single FEL pulse. Here, we aim to shed light on the following questions inherent FEL and synchrotron experiments: a) whether the resolution achievable on a single feature is hampered by the feature embedded in a larger object, and b) whether different imaging techniques exhibit different efficiency. To address these issues, we present a signal-to-noise criterion, based on a Gaussian scatterer model, which predicts whether a feature of a given size and scattering strength placed inside a larger object can be retrieved with two common X-ray imaging techniques [3]: i) real space projection microscopy (PM) and ii) Fourier space coherent diffraction imaging (CDI).

The proposed criterion, validated quantitatively through simulations, predicts that PM requires less photons per unit of area, i.e., is more sensitive than CDI to identify weaker and smaller features in the aforementioned conditions. The criterion accounts for the size of the full object in which the features are embedded, and predicts deterioration of the imaging performance with increasing the object size, which is in contrast with previous studies. The criterion can be applied to optimize the design of imaging experiments at FEL and synchrotron facilities.

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XFEL Serial Crystallography of Fibrous Specimens

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ABSTRACT

The most successful application of XFELs so far, at least as far as structural biology is concerned, has been in serial femtosecond nanocrystallography [1,2]. The high intensity and short pulse duration allows collection of hundreds of thousands of diffraction patterns from tiny crystals without radiation damage. However, crystallinity is an artifice to increase signal strength and assist in orienting the patterns in reciprocal space. The use of single particles would provide data with more information and would simplify phasing. Although some progress has been made, single particle imaging is plagued by low signal levels and difficulties with orienting the data, and success so far has been limited to low resolution. Fibrous assemblies, that are periodic along one axis but exhibit little or no crystallinity in the plane lateral to this axis, are intermediate between 3D crystals and single particles, and are thus an interesting target for XFEL studies. Furthermore, fibrous molecules and assemblies are ubiquitous in biology, with their fibrous nature often being key to their biological function. Traditionally, these kinds of molecules have been studied by "x-ray fiber diffraction." Indeed, such studies were important in early work on nucleic acids, fibrous proteins, polysaccharides, helical viruses and microtubules [3]. However, fiber diffraction analysis has limited scope in general, because the specimen is rotationally disordered and the diffraction is cylindrically averaged, drastically reducing the information content of the diffraction data. XFELs open up new opportunities for studying fibrous molecules and assemblies, utilizing flow alignment, a highly focused x-ray pulse, and signal enhancement due to the one-dimensional periodicity, to potentially collect data from single fibers. We have conducted experiments at the CXI station at the LCLS with a number of fibrous systems. With an amyloid-forming oligopeptide, the diffraction data show good flow alignment, and signal strength enhanced by the axial periodicity and some limited lateral crystallinity. The data is first processed to detect likely single hits (the x-ray pulse intersecting a single fiber). Although the patterns are sparse and weak, their analysis allows two degrees of freedom in the fiber orientation to be estimated. Subsequent analysis allows the third degree of freedom to also be estimated. With the particle orientation determined, there is the possibility of mapping full 3D reciprocal space, overcoming the primary the limitation of cylindrical averaging in conventional fiber diffraction. The nature of the data obtained and the processing methods developed will be described. The experiments described here were conducted as part of a large collaboration between investigators at UC, CFEL, LCLS and ILL.

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Coherently Focused Beam Waist Characterized by Ptychography and Speckle Analysis

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ABSTRACT

Last advances in the development of 3rd generation synchrotrons towards diffraction limited sources provide excellent conditions for exploring spatially coherent X-ray beams. This has led to a rapid development of X-ray photon correlation spectroscopy (XPCS) and lensless coherent diffractive imaging (CDI) techniques, which require that a well-defined phase relation is preserved through the scattering process. When oversampling condition is fulfilled, the coherent diffraction pattern carries the information of the exact arrangement of scatterers constituting a specimen. This enables to study dynamics in disordered materials using XPCS technique based on correlation analysis of temporal fluctuations of scattering patterns ('speckles') [1]. In CDI the coherent diffraction pattern is inverted by iterative phase retrieval algorithms to yield a real space image of an illuminated object. First demonstration of CDI applied to a non-crystalline test object was reported by Miao *et al* [2]. Application to crystalline materials has been demonstrated in pioneering works by Robinson *et al*, where CDI in Bragg geometry was used to image gold nanocrystal [3].

In order to enhance the convergence of phase retrieval in CDI the ptychography technique has been recently devised [4]. In this technique the multiple CDI patterns are collected while a sample is scanned across the localized probe beam with spatial overlap between adjacent positions. Ptychographic CDI have recently emerged as a technique with great potential for 3D imaging of biological specimens [5] as well as determination of atomic displacement fields inside nanocrystals [6].

When a strongly scattering calibration object is used, the ptychography data enable to retrieve both object transmission and probe complex-valued wavefields. This provides excellent means for characterization of coherent beams produced by focusing optics at 3rd generation synchrotron sources and free-electron laser facilities. While the common trend is to use nanofocused beams, exploiting focused beams of medium-size (several microns) represent certain advantages in terms of illuminated field of view and less demanding conditions for stability and scanning resolution.

We report here on the characterization of the focal waist of micron-size beams produced by compound refractive lenses (CRL) at the P10 coherence beamline of PETRA III synchrotron source at DESY Hamburg. Using ptychography, the full 3D characterization of the wavefield distribution at the CRL beam waist as well as test object reconstruction have been performed. The details of optimization of coherent illumination via speckle contrast measurement will be also discussed.

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