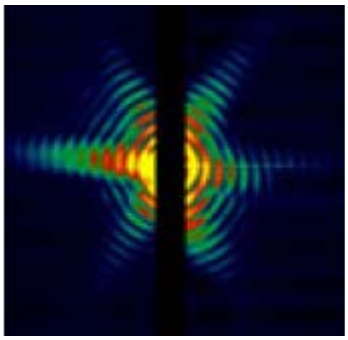
Book of Abstracts

COHERENCE 2010



Welcome to Warnemünde

On behalf of the Organizing Committee and the International Program Committee I would like to welcome you to *Coherence 2010, the International Workshop on Phase Retrieval and Coherent Scattering.* This is the fifth meeting, in what is becoming a very popular series of workshops, in the application and study of coherent wavefields, particularly at short wavelengths. The field of research goes by many names and descriptions: the phase problem, correlations and speckle, the extension of crystallography to non-periodic objects, or simply coherent X-ray and electron science.

The field is actually quite old: the theory of crystal diffraction laid down by von Laue almost 100 years ago assumes complete spatial coherence, which is indeed the case over the unit cell dimensions of crystals placed any practical distance from an X-ray tube. Developments in electron imaging and coherent visible optics led to techniques and algorithms for overcoming the phase problem for non-periodic objects, which were tried out on modern high-brightness electron and X-ray sources. Over the last decade, since the first workshop organized by John Spence in 2000, we have made great progress in closing the gap between the wonderful possibilities suggested by experiments in the computer and the achievements of experiments. Today, X-ray free-electron lasers are a reality, bringing fully coherent ultrafast pulses. With them come even more fantastic ideas of how to utilize coherent wavefields and extract structural information at atomic times and distances, and fuelling the growth and impact of the field.

The past workshops were in Berkeley (2000), Cairns (2003), Porquerolles (2005), and Asilomar (2007). This year we followed the well-established tradition of a sear location, and in encouraging people to stay at the hotel to ensure plenty of informal discussion time and interactions. Our site is at the highest latitude yet of the series, which brings the benefit of long daylight hours, as long as the clouds remain out of view. In any case, the Baltic Sea offers many delights to complement the great science that will be discussed.

I would like to acknowledge the financial support of DESY, the European XFEL GmbH, and TU Berlin, as well as that of our sponsors. I would also like to thank the efforts of the local organizing committee as well as the program committee in putting together an exciting schedule.

I hope you have a great time here in Warnemünde.

Henry Chapman.

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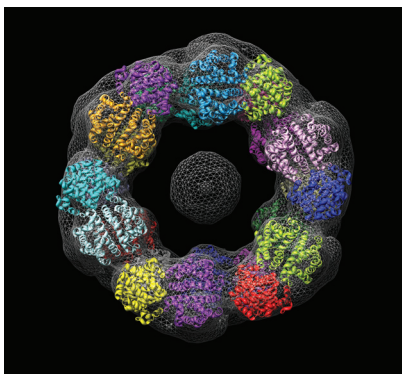

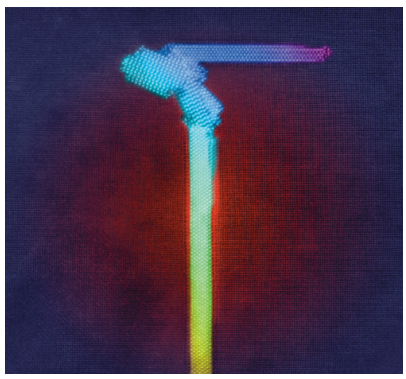

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	Tuesday, 8th June	Wednesday 9th June	Thursday, 10th June	Friday, 11th June
		CORRELATIONS & OPTICS Chair: Salditt	XPCS II Chair: Madsen	PHASING METHODS Chair: Robinson
09.00		Gutt: Detecting and quantifying local symmetries in disordered materials via speckle fluctuations	Leheny: Connecting Nanoscale Motion and Rheology of Viscoelastic and Glassy Complex Fluids	Shpyrko / Mc Nulty: Imaging Magnetic Structure by Coherent X-ray Diffraction
09.40		Saldin: Structure from Correlated Scattering	Mueller: Atomic dynamics at the martensitic phase transition of Au-Cd by X-ray Photon Correlation Spectroscopy	Zhang: A robust coherent imaging approach based on wavefront modulation
10.00			Chushkin: Dynamics of concentrated suspensions of nanoparticles in supercooled liquids	Itoh: Two-dimensional grating-based X-ray phase-contrast imaging with Fourier transform phase retrieval
10.20		Mimura: Development of an adaptive optical system for hard X-ray nanofocusing	Robert: The X-ray Correlation Spectroscopy Instrument at the Linac Coherent Light Source : Status and Perspectives	Guizar-Sicairos: Development of a Novel Holography Technique for X-ray Coherent Diffractive Imaging
10.40			Coffee Break	Coffee Break
			3 D DIFFRACTIVE IMAGING Chair: Jacobsen	FEL-BASED IMAGING Chair: Kirz
11.00		Coffee Break	Steinbrener: X-ray Diffraction Microscopy of Frozen-Hydrated and Freeze-Dried Eukaryotic Cells	Maia: Single Shot 3D Imaging of Sparse System using Compressed Sensing
		XPCS I Chair: Tschentscher		
11.20		Leitner: Following atomic dynamics using coherent X-rays		
11.40			Lima: Cryogenic x-ray diffraction microscopy for biological samples	Quiney: Determination of biomolecular structures using fourth-generation X-ray sources
12.00		Fluerasu / Madsen: Catching the dynamics on the go: Recent X-ray Photon Correlation Experiments with flowing samples	Robinson: Shape-dependent chemical-induced strains in gold nanocrystals	Williams: An instrument for nanocrystal diffraction and imaging at the LCLS
12.20		Lunch	Chamard: Three-Dimensional X-ray Fourier Transform Holography: the Bragg Case	Pfau: Ultrafast Resonant Magnetic Scattering at the Free-Electron Laser FLASH
12.40			Lunch	Bornath: Dense Xenon Nanoplasmas in Intense Laser Fields
12.50				
01.00				CLOSING REMARKS
		PTYCHOGRAPHY Chair: Pfeiffer		
01.20		Dierolf: Recent developments in ptychographic coherent diffractive imaging		Lunch & Departure
02.00		Giewekemeyer: Quantitative Biological Imaging by Ptychographic X-ray Diffraction Microscopy	Free Afternoon	
02.20		Thibault:: Ptychography in the weakly scattering limit		
02.40		Gührs: Wavefield Back-Propagation in High-Resolution X-ray Holography with a Movable Field of View		
03.00		Coffee Break		
		COHERENT ELECTRON DIFFRACTION Chair: Mimura		
03.20		Dronyak: Three-Dimensional Coherent Electron Diffractive Imaging of a Single Nanocrystal		
04.00	Registration	Yamasaki: Reconstruction of Crystalline Structures at 78 pm Resolution by Electron Diffractive Imaging		
04.20		Luiten: Single-shot Femtosecond Electron Diffraction		
05.00	Welcome			
	COHERENCE Chair: Grübel			
05.20	Nugent: Partial Coherence, Phase Diversity and Coherent X-ray Imaging			
06.00	Sinha: Dynamical Studies using Coherent X-Rays: A short review and prospects for the future	Dinner		
06.40	Kirz: Plans for a soft X-ray FEL for dynamic imaging			
07.00	Welcome Reception	Poster Session		
07.50			07.45 Dinner (Banquet)	
08.30				

Oral Presentations

Coherence

Chair: *Gerhard Gruebel*

8th June, 5.20 p.m. – Invited Speaker

Partial Coherence, Phase Diversity and Coherent X-ray Imaging

Prof. Keith Nugent

The University of Melbourne

The coherent output of modern X-ray sources continues to grow rapidly. However, even with X-ray free electron laser sources, the beam is not fully coherent. In this presentation, I show how one can properly characterise the coherence of an X-ray beam and include these properties into the image recovery methodology for coherent diffractive imaging (CDI). Methods have been experimentally demonstrated for the cases of both imperfect temporal and spatial coherence. We find that the increase in the acceptable phase-space of the incident radiation has the potential to significantly reduce exposure times for CDI. If time permits, I will also introduce the concept of phase-diversity for coherent X-ray imaging and show some examples of its application to a biological imaging problem.

8th June, 6.00 p.m. – Invited Speaker

Dynamical Studies using Coherent X-Rays: A short review and prospects for the future

Prof. Sunil Sinha

University of California San Diego

The field of X-ray Photon Correlation Spectroscopy has steadily grown from "demonstration" experiments about 15 years ago, to studies addressing real problems at the forefront of condensed matter, and has attracted increasing numbers of users. The principal applications have been in the field of soft condensed matter and nanoscience, but the extension to the study of slow fluctuations in magnetic systems will undoubtedly grow. The most frequent limits which experimenters run up against are coherent intensity, long-term stability of the beam, radiation damage, and extension of the time window to very short or long times and to larger wave vector transfers. In this talk, I will attempt to survey some of the recent applications which are at the limits of currently existing instruments, and present a wish list for XPCS-capable beamlines of the future for attacking certain important problems in condensed matter and materials science. I will also discuss some developments in coherent scattering, excluding imaging and phase retrieval studies.

8th June, 6.40 p.m.

Plans for a soft X-ray FEL for dynamic imaging*

John Corlett, Peter Denes, Roger Falcone, Janos Kirz, Robert Schoenlein

Lawrence Berkeley National Laboratory

Experiments at FLASH and at LCLS have amply demonstrated the power of free electron lasers to perform imaging experiments using ultrashort pulses. The coherence of the source, the ability to capture an image before radiation damage manifests itself, and to observe phenomena on the femtosecond time scale has opened up a broad array of microscopy applications The sample is usually destroyed by a single FEL pulse in these experiments. In order to do systematic dynamical studies on the same sample, one needs a more gentle probe, and one that operates at high repetition rates. At Lawrence Berkeley Laboratory an array of high rate soft X-ray FEL-s is being designed [1] that will be ideally suited for the study of dynamics on time scales from a fraction of a femtosecond to milliseconds. The transform-limited coherent beams will be fully tunable up to 1.2 KeV in the fundamental, and up to 6 KeV (at reduced fluence) in the higher harmonics. The pulse-rate will be user-selectable with complete flexibility up to 100 KHz or even higher.

[1] J. Corlett et al., Synchrotron Radiation News 22 No5, 25 (2009)

*Supported by the Office of Basic Energy Sciences, US Department of Energy

Correlation & Optics

Chair: *Tim Salditt*

9th June, 9.00 a.m. – Invited Speaker

Detecting and quantifying local symmetries in disordered materials via speckle fluctuations

Dr. Christian Gutt[1], Dr. Peter Wochner[2], Dr. Birgit Fischer[1], Dr. Miguel Castro Colin[2], Dr. Gerhard Grübel[1]

[1]DESY
[2] Max-Planck Institute, Stuttgart

Disordered matter –such as liquids and glasses – does not exhibit long range translational order and in turn is able to accommodate different local symmetries in the same system. Local structures have always been fascinating to scientists because they are held responsible for the undercooling of liquids and the existence of the glassy state. Moreover, non periodic materials have always attracted the attention of materials scientists, because they do carry, through their structural degrees of freedom, a unique potential to display smart functions. However, the local microscopic structure of disordered structures has remained a challenge and a mystery. Conventional X-ray diffraction techniques fail to detect local structures because of their intrinsic spatial and temporal averaging mechanism. Our lack of knowledge on local order within disorder constrains the development of an understanding of the properties of liquids and glasses. Therefore, the question how those structures can be accessed experimentally has become one of the holy grails of condensed matter science. The guiding principle to solve this problem is to avoid temporal and spatial averaging by using coherent X-rays [1]. The resulting speckle pattern of a liquid/glass reflects the exact spatial arrangement of all the particles in the beam and allows to test for local order. We show with the help of computer simulations how to construct proper speckle correlators and use statistical averages to detect and quantify local symmetries in disordered matter [2]. The newly developed techniques are employed to experimental data from colloidal glasses.

[1] P. Wochner, C. Gutt, T. Autenrieth, T. Demmer, V. Bugaev, A. Diaz Ortiz, A. Duri, F. Zontone, G. Grubel and H. Dosch, PNAS 106, 11511 (2009)
[2] C. Gutt et al. submitted

9th June, 9.40 a.m. – Invited Speaker

Structure from Correlated Scattering

Prof. Dilano Saldin[1], Dr. Hin-cheuck Poon[1], Dr. Malcolm Howells[2], Prof. Henry Chapman[3], Mr. Richard Kirian[4], Prof. John Spence[4]

[1]Department of Physics, University of Wisconsin-Milwaukee
[2]Lawrence Berkeley National Laboratory
[3] DESY and University of Hamburg
[4]Arizona State University

The average angular correlations from diffraction patterns of identical particles in different orientations tend towards a reproducible signal which may be decoded to reconstruct a single-particle diffraction pattern from measured scattering by many particles in random orientations [1,2]. Measurements of intensity correlations therefore allow a single-particle diffraction pattern to be extracted from multiparticle scattering. We describe potential applications to structure determination from unaligned particles in e.g. liquids or cell membranes [3,4] as well as in molecular beams illuminated by radiation from an x-ray free electron laser (XFEL) [2]. Such methods remove the need for crystallization while retaining the advantages of signal amplification by scattering from many identical particles. A real space image may be obtained from the reconstructed diffraction pattern in the usual way by an iterative phasing algorithm, e.g. [5]. We will also discuss a possible application to measurement of time-resolved structural changes of single molecules [2,6].

[1] Z. Kam, Macrocolecules 10, 927 (1977).
[2] D. K. Saldin et al., J. Phys: Condens. Matter 21, 134014 (2009).
[3] D. K. Saldin et al., New J. Phys. 12, 035014 (2010).
[4] D. K. Saldin et al., Phys. Rev. B 81, 174105 (2010).
[5] G. Oszlanyi and A. Suto, Acta Cryst A60, 134 (2004).
[6] J. C. H. Spence et al., Microscopy and Microanalysis Meeting, Portland (2010).

9th June, 10.20 a.m. – Invited Speaker

Development of an adaptive optical system for hard X-ray nanofocusing

Dr. Hidekazu Mimura, Prof. Kazuto Yamauchi

Osaka University

Hard X-rays have extremely short wavelengths corresponding to the atomic spacing of materials. These short wavelengths allow hard X-rays to be confined within nanometer-sized areas. This conceptually simple but technically difficult idea has lead to a large degree of interest in methods of X-ray focusing. In this presentation, we will propose a method for approaching sub-10nm sized hard X-rays using an adaptive optical system. Phase retrieval calculations are employed to determine wavefront distortions of the focused beam. The grazing incidence deformable mirror restore the wavefront shape. Even if hard X-ray focusing elements do not achieve sufficient performance, the ideal focusing condition is obtainable. This rational system with X-ray nanobeam will enable diffraction-limited spatial resolution in various X-ray analytical methods.

XPCS - I

Chair: *Thomas Tschentscher*

9th June, 11.20 a.m. – Invited Speaker

Following atomic dynamics using coherent X-rays

Michael Leitner

Universität Wien

X-ray photon correlation spectroscopy (XPCS) is a comparatively new technique, allowing to study slow dynamics of condensed matter. Because of the X-rays' wavelengths, the accessible length scales are commonly given as reaching the Å-range. Experimental confirmations of this claim have been lacking, however, mainly because of the minute amounts of scattered radiation at high scattering angles under coherent conditions. Only recently we have been able to demonstrate the possibility to study atomic dynamics, i.e. to experimentally ascertain the direction, length, and frequency of the atomic jumps, by doing XPCS at existing X-ray sources [1]. The sample is an alloy single crystal. The information about atomic dynamics is encoded in the temporal variations of the scattered intensity in the diffuse regime, i.e. away from Bragg peaks, which is due to the statistical occupancy of the lattice sites by the different species of atoms. The necessary scattering angles are typically more than 20°. Ensuring a partially coherent beam with a coherence factor of a few percent, the detected intensity is on the scale of a few photons per pixel and hour. I will first give a quick overview of the concepts and the theoretical background of diffusion on a lattice, and I will then present our results on the atomic jumps in the short-range ordered alloy Cu-10at.%Au and preliminary results on diffusion in a metallic glass. I will comment on the data evaluation given above-mentioned low count rates and on the limits of accessible systems in terms of scattered intensity.

[1] M. Leitner, B. Sepiol, L.-M. Stadler, B. Pfau, and G. Vogl, Nature Mat. 8, 717 (2009).

9th June, 12.00 a.m.

Catching the dynamics on the go: Recent X-ray Photon Correlation Experiments with flowing samples

Dr. Andrei Fluerasu[1], Dr. Anders Madsen[2]

[1]Brookhaven National Laboratory, NSLS-II
[2]European Synchrotron Radiation Facility, B.P. 220, F-38043 Grenoble, France

X-ray Photon Correlation Spectroscopy (XPCS) has emerged as a unique technique allowing the measurement of dynamics in materials on mesoscopic length scales. One of the most common problems associated with the use of bright X-ray beams is beam-induced radiation damage, and this is clearly going to be an even more limiting factor at future Synchrotron and Free Electron Laser (FEL) sources. Flowing the sample during acquisition is one of the simplest methods allowing to limit the radiation damage. In addition to distributing the dose over many different scatterers, the method also enables new functionalities (e.g. time-resolved studies). One of the important problems appearing in an experiment with a "moving sample" is associated with the fact that the dissipative dynamics and the advective response to shear are convoluted in a non-trivial way in the measured correlation functions.In this talk, I will describe some recent results in which we show how the macroscopic advective response to flow and the microscopic diffusive dynamics can both be quantified from the XPCS data. I will also discuss the effect that the applied shear may have on the diverging short-time and long-time relaxation rates in high density colloidal suspensions. All these results will be discusses in view of other on-going and future projects, including experiments at new light sources such as NSLS-II and the FELs.

Ptychography

Chair: *Franz Pfeiffer*

9th June, 1.20 p.m. – Invited Speaker

Recent developments in ptychographic coherent diffractive imaging

Mr. Martin Dierolf[1], Dr. Pierre Thibault[1], Dr. Andreas Menzel[2], Dr. Cameron M. Kewish[2], Dr. Oliver Bunk[2], Prof. Franz Pfeiffer[1]

[1]Department of Physics (E17), Technische Universität München, Garching, Germany
[2]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Applying iterative phase retrieval schemes to ptychographic data, i.e., diffraction patterns collected with a localized illumination probe from overlapping regions of a specimen, has enabled the investigation of non-isolated, extended specimens previously inaccessible by other coherent X-ray diffractive imaging (CDI) methods [1]. Recent algorithmic developments allow now the simultaneous reconstruction of both probe and object [2-5] and thus overcome the initial limitation of requiring precise knowledge of the illumination function. Together with schemes to suppress an inherent ambiguity [6], this paves the way not only to routine combination of ptychographic CDI with X-ray scanning microscopy methods, but also towards investigations of three-dimensional specimens. We will present our recent work on imaging optically-thick three-dimensional specimens by means of nanotomography based on ptychographic CDI. Examples include the reconstruction of the high-contrast quantitative three-dimensional electron density map of a mouse femur sample.

[1] J. M. Rodenburg, A. C. Hurst, A. G. Cullis, B. R. Dobson, F. Pfeiffer, O. Bunk, C. David, K. Jefimovs, I. Johnson, Phys. Rev. Lett. 98, 034801 (2007).
[2] P. Thibault, M. Dierolf, A. Menzel, O. Bunk, C. David, F. Pfeiffer, Science 321, 379 (2008).
[3] M.Guizar-Sicairos, J. R. Fienup, Opt. Express 16, 7264 (2008).
[4] A. M. Maiden, J. M. Rodenburg, Ultramicroscopy 109, 1256 (2009).
[5] K. Giewekemeyer, P. Thibault, S. Kalbeisch, A. Beerlink, C. M. Kewish, M. Dierolf, F. Pfeiff er, T. Salditt, PNAS 107, 529 (2009).
[6] M. Dierolf, P. Thibault, A. Menzel, C. M. Kewish, K. Jefimovs, I. Schlichting, K. von Koenig, O. Bunk, F. Pfeiffer, New Journal of Physics 12, 035017(2010).

9th June, 2.00 p.m.

Quantitative Biological Imaging by Ptychographic X-ray Diffraction Microscopy

Klaus Giewekemeyer[1], Pierre Thibault[2], Sebastian Kalbfleisch[1], André Beerlink[1], Cameron M. Kewish[3], Martin Dierolf[1], Franz Pfeiffer, Tim Salditt[1]

[1]Institut für Röntgenphysik, Georg-August-Universität Göttingen
[2]Department of Physics (E17), Technische Universität München, Garching, Germany
[3]Synchrotron SOLEIL

Ptychographic Diffractive Imaging has proved itself a very powerful tool in coherent X-ray imaging as it enables observations with an unlimited field of view and is characterized by fast convergence and a low degree of ambiguity in the reconstruction [1]. Recently it was shown experimentally that a pre-knowledge of the complex illuminating wavefield in the sample plane is not necessary any more, but can self-consistently be recovered together with the object transmission function from the same dataset [2]. In this contribution we will report on one of the first applications of this new technique to unstained biological specimens, namely freeze-dried cells of the procaryotic bacterium Deinococcus radiodurans, which have been imaged at the cSAXS beamline of the Swiss Light Source using a pinhole (diameter 1.4 microns) as the beam-defining optical element at a photon energy of 6.2 keV. We will show how quantitive phase information with a sensitivity better than 0.03 rad can be extracted from the data which has been phased down to a resolution below 100 nm (half-period length), according to an analysis of the phase retrieval transfer function and the power spectral density of the reconstructed phase map. During the scan with highest resolution a cell was exposed to the relatively low dose of 1.3*10^5 Gy. Finally, projected mass density maps with small and quantified errors could be extracted from the phase distributions, as no beamstop was used and the total amount of photons impinging on the sample could be detected with the single-photon counting PILATUS detector.

[1] Rodenburg, J.M., et al. Phys. Rev. Lett. 98 (2007) 034801.
[2] Thibault, P., et al. Science 321 (2008) 379.
[3] Giewekemeyer,K. et al., P.N.A.S. 107 (2010) 529-534.

9th June, 2.20 p.m.

Ptychography in the weakly scattering limit

Dr. Pierre Thibault[1], Mr. Martin Dierolf[1], Dr. Cameron M. Kewish[2], Dr. Andreas Menzel[3], Dr. Oliver Bunk[3], Prof. Franz Pfeiffer[4]

[1]Technical University of Munich
[2]Synchrotron SOLEIL
[3]Paul Scherrer Institut
[4]Technical University of Munich

The last few years have seen a few demonstrations that ptychography can eliminate some of the most limiting downsides of the classical version of diffraction microscopy. Among other benefits, the possibility of imaging extended specimens is probably the most remarkable. In addition, most reconstruction procedures currently available are fast, straightforward and reliable. In face of these successes, it is fair to ask where are the trade-offs. Apart from the obvious fact that ptychography is not immediately compatible with "single-shot" measurements (especially when the single shot damages the sample), we will discuss the important implications of departure from a plane-wave illumination, and the reliance on a scanning system. For instance, imaging weakly scattering structures seems at first sight especially difficult because diffraction of a non-planar illumination necessarily encroaches on the weak scattering from the specimen (we will show that in fact this is not a limitation). Accumulating sufficient statistics from weak specimens also requires longer exposure times, thus increasing the sensitivity to various mechanical instabilities. Solutions to these types of problems will be presented and demonstrated with simulated and real data.

9th June, 2.40 p.m.

Wavefield Back-Propagation in High-Resolution X-ray Holography with a Movable Field of View

Mr. Erik Guehrs[1], Christian Günther[2], Bastian Pfau[1], Torbjörn Rander1, Stefan Schaffert[1], William Schlotter[3], Stefan Eisebitt[1]

[1]Technische Universität Berlin
[2]Helmholtz-Zentrum berlin
[3]Centre for Free-Electron Laser Science, Universität Hamburg

Mask-based Fourier transform holography (FTH) is used to record images of biological objects with 2.2 nm X-ray wavelength. The holography mask and the object are separated from each other allowing us to move the field of view of the sample. Due to the separation of the holography mask and the sample on different X-ray support membranes, a gap between both windows of several 10s of microns typically exists which can be due to misalignment or dust or is desired to protect the sample from direct contact with the holography mask. In particular, in high-resolution imaging with soft X-rays the depth of field, thus limits the gap size for which sharp images of the sample can be reconstructed using a 2D Fourier Transform of the hologram. In this contribution, we systematically investigate the imaging and reconstruction conditions for mask-sample separations up to 400 μm. With holograms from diatom samples at variable gap distance, we demonstrate the feasibility to combine FTH and wavefield back-propagation to obtain a focused image even for the largest separations. We discuss the limitations of our approach which are mainly associated with the Fresnel illumination function of the object. In particular for high-resolution imaging with soft X-rays and the associated small fields of view below 2 μm, our approach is crucial in order to obtain diffraction limited resolution combined with experimental ease regarding the scanning setup.

Electron Diffraction

Chair: *Hidekazu Mimura*

9th June, 3.20 p.m. – Invited Speaker

Three-Dimensional Coherent Electron Diffractive Imaging of a Single Nanocrystal

Mr. Roman Dronyak[1,2], Dr. Keng S. Liang[1], Dr. Ting-kuo Lee[3], Prof. Fu-rong Chen[2]

[1]National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu 30076, Taiwan
[2]Department of Engineering and System Science, National Tsing Hua University, Hsinchu 30013, Taiwan
[3]Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan

Coherent diffractive imaging (CDI) with electron or x-ray sources is a promising technique for investigating the structure of nanoparticles down to the atomic scale. For electron CDI, a two-dimensional reconstruction has been demonstrated [1-3]. Here, for the first time, we have experimentally determined a three-dimensional (3D) morphology of a single MgO nanocrystal using electron CDI in the Bragg diffraction geometry [4]. In the experiment, we used a JEOL 2010F electron microscope equipped with a field-emission gun providing a highly coherent nano-sized electron beam. In our data analysis, we have used a guided hybrid input-output algorithm with a shrink-wrap method [3]. The result of the reconstruction shows that the recorded continuous 3D diffraction pattern around the (200) reflection of the nanoparticle reveals a 3D shape of the sample, which is consistent with simulation. Measuring the intensity over the angular range of 1.8 degrees provides a spatial resolution of about 8 nm along the direction of the electron beam propagation.
Our results demonstrate a new way of obtaining the 3D structure of nanoparticles, different from conventional tomography methods used in electron microscopy. The experiment, diffraction geometry, reconstruction procedure and multiple scattering effects will be discussed in details.

[1] J. M. Zuo, I. Vartanyants, M. Gao, R. Zhang, and L. A. Nagahara, Science 300, 1419 (2003).
[2] W. J. Huang, J. M. Zuo, B. Jiang, K.W. Kwon, and M. Shim, Nat. Phys. 5, 129 (2009).
[3] R. Dronyak, K. S. Liang, Y. P. Stetsko, T. K. Lee, C. K. Feng, J. S. Tsai, and F. R. Chen, Appl. Phys. Lett. 95, 111908 (2009).
[4] G. J. Williams, M. A. Pfeifer, I. A. Vartanyants, and I. K. Robinson, Phys. Rev. Lett. 90, 175501 (2003).

9th June, 4.00 p.m.

Reconstruction of Crystalline Structures at 78 pm Resolution by Electron Diffractive Imaging

Dr. Jun Yamasaki, Mr. Shigeyuki Morishita, Prof. Nobuo Tanaka

Nagoya University

Since the first high-resolution reconstruction in 2003 [1], electron diffractive imaging has drawn the attention as a new imaging method in the field of electron microscopy. One of the notable merits of the electron diffractive imaging is that spatial resolutions in reconstructed images are not limited basically by lens aberrations in transmission electron microscopes (TEM). The method was, however, available only for samples isolated in empty space such as nanotubes and nanowires. In order to avoid the restriction, we have proposed a new procedure available for thin film samples by using an aperture in an aberration-corrected TEM [2]. Reconstruction of a thin crystalline film with an atomic resolution was demonstrated using the Si <011> dumbbell structure with the separation of 136 pm [3]. In this study, we have tried to achieve a higher resolution than that in high-resolution TEM, which is limited to about 100 pm in 200 kV instruments. Using a [112] diffraction pattern from a Si crystal, we have succeeded in clear imaging of atomic columns with the separation of 78 pm, which is the highest resolution ever reported on diffractive imaging. Identification of different elements in a compound has been also examined using a MgO crystal. From a [011] diffraction pattern, Mg and O columns have been clearly reconstructed as different intensities. The above results confirm the high-resolution ability and the availability of our method, which shows promise as a new imaging method for atomic structures in materials.

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9th June, 4.20 p.m. – Invited Speaker

Single-shot Femtosecond Electron Diffraction

Dr. Jom Luiten

Eindhoven University of Technology

Electrons and X-rays both enable the study of structural dynamics at atomic length scales, but the nature of their interaction with matter is entirely different. As a consequence, the information that can be extracted by probing with either electrons or X-rays is quite different and, in fact, complementary. A pulsed electron source with the X-ray Free Electron Laser capability of performing single-shot, femtosecond diffraction would therefore be highly desirable. The primary obstacle facing the realization of such an electron source is the space charge problem: packing the number of electrons required for recording a full diffraction pattern in a single sub-ps pulse will inevitably lead to a rapid Coulomb expansion of the pulse and therefore loss of temporal resolution. We have developed a method, based on radio-frequency (RF) techniques, to invert the Coulomb expansion. We will report on the first experiments demonstrating RF compression of 0.25 pC, 100 keV electron bunches to 100 fs bunch lengths. We have used these bunches to produce high-quality, single-shot diffraction patterns of poly-crystalline gold. In all ultrafast electron diffraction experiments up to now electron bunches have been generated by femtosecond photoemission from metal cathodes. The transverse coherence length of the resulting beams is fundamentally limited to ~1 nm for crystal samples of ~100 micron size, and therefore does not allow the study of, e.g., protein samples. We have developed a new, ultracold pulsed electron source, based on near-threshold photo-ionization of a laser-cooled gas. The source is characterized by an effective electron temperature of ~10 K, almost three orders of magnitude lower than conventional sources. This should enable coherence lengths of a few tens of nm for crystal samples with a size of ~100 micron. By combining the ultracold electron source with RF acceleration and bunch compression techniques, single-shot, sub-ps studies of the structural dynamics of macromolecular crystals will become possible.

XPCS - II

Chair: *Anders Madsen*

10th June, 9.00 a.m. – Invited Speaker

Connecting Nanoscale Motion and Rheology of Viscoelastic and Glassy Complex Fluids

Mr. Hongyu Guo[1], James Harden[2], Subramanian Ramakrishnan[3], Gilles Bourrey[4], R. Bruce Lennox[4], Mark Sutton[4], Robert Leheny[1]

[1]Johns Hopkins University
[2]University of Ottawa
[3]Florida State University
[4]McGill University

Complex fluids -- such as colloidal suspensions, polymers, and surfactant solutions -- often display complicated mechanical properties that derive from the dynamics of their internal structure on the nanometer or micrometer scale. However, connecting these macroscopic and microscopic behaviors can be difficult and remains a central challenge to understanding such materials. The development of x-ray photon correlation spectroscopy (XPCS) has created new opportunities to probe slow, nanoscale dynamics in complex fluids. In this talk, I will discuss two examples, glassy colloidal gels and viscoelastic polymer solutions, in which the combination of XPCS and rheology provides connections between the microscopic and macroscopic.

10th June, 9.40 a.m.

Atomic dynamics at the martensitic phase transition of Au-Cd by X-ray Photon Correlation Spectroscopy

Dr. Leonard Mueller[1], Mr. Moritz Waldorf[2], Dr. Christian Gutt[1], Dr. Gerhard Grübel[1], Dr. Anders Madsen[3], Prof. Trevor R.Finlayson[4], Prof. Uwe Klemradt[2]

[1] HASYLAB @ DESY
[2] II. Physikalisches Institut, RWTH Aachen University
[3]ESRF, Grenoble
[4]School of Physics, University of Melbourne

Aging phenomena of martensites have been discussed controversially for decades. Although they were successfully associated with defect related diffusion processes in the low temperature (martensite) phase (Ren and Otsuka, Nature 389, 579 (1997)), so far no experiments have addressed in-situ the characteristic time scales associated with the nanoscopic structural changes. Using a Au50.5Cd49.5 single crystal, X-ray photon correlation spectroscopy (XPCS) measurements in diffraction geometry were carried out at ESRF beamline ID10A. High temperature resolution (0.1K) and stability (±4mK) were employed to resolve potential slow dynamics in the vicinity of the phase transition, 2D scattering data close to the (001) Bragg reflection were recorded with a sampling time of 0.2 s at 1.4 s intervals. Significant dynamics are only observed near the martensite start temperature, Ms, which indicates the beginning of the phase transformation. Being fastest at the transition, the measured dynamics are in disagreement with any critical slowing down scenario suggested previously. At the transition temperature the two-time correlation function reveal a non-stationary behaviour and also avalanches in the sample. Characteristic timescales were determined as a function of the aging-time by calculating one-time-correlation functions at a specific age. The two-time correlation function additionally shows the transition from strain dominated dynamics to a diffusive or even glassy behaviour of the sample.

10th June, 10.00 a.m.

Dynamics of concentrated suspensions of nanoparticles in supercooled liquids

Dr. Yuriy Chushkin[1], Dr. Chiara Caronna[2], Dr. Anders Madsen[3]

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Using tracer particles is a common technique to study the rheological and dynamical behavior of complex fluids in which the tracers are suspended. Recently, this strategy was successfully applied to investigate the dynamical properties of a glass forming liquid in the supercooled state by X-ray photon correlation spectroscopy (XPCS) [1]. It was found that the dynamics of silica nano-particles suspended in propanediol (PG) change character upon approaching glass transition temperature (Tg) of PG. Down to about 215 K (1.26Tg), the particles undergo Brownian motion as expected for this dilute suspension but at lower temperatures they show hyper-diffusive behavior. This change was observed 40-50 K above Tg of the solvent and it could be associated either with the rugged potential energy landscape of the fragile glass-former PG or with dynamics governed by stress relaxations. The onset of ballistic motion in a system of dilute, non interacting particles suggests the presence of a preferential direction of motion triggered by the supercooled solvent, that would also cause neighboring particles to move cooperatively. This effect should be particularly visible in concentrated suspensions. Molecular dynamics simulations have indicated that the morphology and size of the tracer particles have a profound effect on their dynamics [2] and in this work we investigate the size and concentration dependent dynamics of tracer particles in different glass-formers by XPCS. In addition to the transition to hyper-diffusive motion as previously described, the dynamics also becomes anisotropic and hence depends not only on the magnitude but also on the direction of the momentum transfer (Fig. 1). The observed dynamical anisotropy does not depend on the particle size nor on the supercooled liquid of choice, but its strength correlates with the particle concentration and the momentum transfer.

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10th June, 10.20 a.m.

The X-ray Correlation Spectroscopy Instrument at the Linac Coherent Light Source: Status and Perspectives

Dr. Aymeric Robert[1], Dr. Chiara Caronna[2], Dr. Sooheyong Lee[1,3]

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[3]DESY

The X-ray Correlation Spectroscopy Instrument (XCS) is one of the four hard x-ray experimental station to be operated at the Linac Coherent Light Source, the world's first hard x-ray free electron laser. The XCS instrument is designed to take full advantage of the unique properties of the LCLS to probe dynamical phenomena in condensed matter systems down to nanometric lengthscales by means of X-ray Photon Correlation Spectroscopy and Coherent Diffraction. The XCS instrument will use the unprecedented coherence and flux properties of the LCLS. It will enable to probe both slow (i.e. with a characteristic time scales larger than 10ms) and ultrafast dynamics (i.e. ranging between hundreds of femtoseconds up to several nanoseconds) in various scattering geometries (SAXS, WAXS, Grazing Incidence). The ultrafast dynamics will use a novel Split and Delay technique. The XCS instrument will soon be accepting proposals at the LCLS (January 2011). This contribution intends to provide the most up to date information about the capabilities of the XCS instrument and to inform users intending to submit proposals.

3D Diffractive Imaging

Chair: *Chris Jacobsen*

10th June, 11.00 a.m. – Invited Speaker

X-ray Diffraction Microscopy of Frozen-Hydrated and Freeze-Dried Eukaryotic Cells

Mr. Jan Steinbrener[1], Ms. Johanna Nelson[1], Mr. Xiaojing Huang[1], Mr. Janos Kirz[2], Mr. Joshua J. Turner[1], Mr. Aaron M. Neiman[1], Mr. Chris Jacobsen[3]

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X-ray diffraction microscopy (XDM) has been successfully employed to a wide variety of samples in 2D and 3D. Working at cryogenic temperatures for biological samples is crucial to minimizing the effects due to radiation damage and it allows for the samples to be imaged in their natural, hydrated state. At the same time it introduces additional complications to the experimental process in order to prevent contamination of the cold sample (which would violate the reconstruction requirement of an isolated sample) and to prevent ice crystals from forming within the cell (which would cause structural damage). Recent results include the first image of a frozen-hydrated eukaryotic cell obtained from diffraction data [1]. Since biological samples are complex systems, immuno-labeling techniques are often used to uniquely identify substructures of interest. We have recently demonstrated molecule specific imaging using immunogold-labeling on a freeze-dried yeast cell to the highest resolution obtained to date for whole eukaryotic cells [2]. Both results represent an important step towards more reliable and readily interpretable x-ray diffraction reconstructions of biological samples. We will discuss details of the experiment and data analysis of recent results and their implications for 3D reconstructions of biological samples.

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[2] J. Nelson et al., Proc. Natl. Acad. Sci., 107, 7235 (2010)

10th June, 11.40 a.m.

Cryogenic x-ray diffraction microscopy for biological Samples

Dr. Enju Lima[1], Dr. Lutz Wiegart[1], Dr. Petra Pernot[2], Dr. Malcolm Howells[3], Dr. Joanna Timmins[2], Dr. Federico Zontone[2], Dr. Anders Madsen[2]

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[3]Lawrence Berkeley National Lab

Imaging of biological material, such as a whole cell, in three dimensions (3D) will deepen our understanding of cellular biology [1]. As we look into cellular organization with high-resolution towards 10 nanometers or below, we begin to see how sub-cellular organelles and macromolecules mutually interact, thus explicating cellular functions. However, as we push the resolution in biological imaging, the challenge becomes how do we preserve samples close to their natural state, especially with thick samples that are not easily accessible by electron microscopy without sectioning them into thin slices. X-ray diffraction microscopy (XDM) utilizes the high penetration power of x-rays to probe thick samples, avoiding needless sample preparation such as plastic embedding and sectioning. It uses a computational algorithm to reach high resolution by phasing a diffraction pattern to a real space image. Thus, it bypasses many hurdles in optics-based imaging such as short depth-of-field and the resolution set by optics. However, XDM is an indirect imaging method that requires high-quality diffraction data to reach a solution. Its previous low success rate with biological samples, especially in the frozen-hydrated state, reflected this problem. However, two groups have recently shown the feasibility of frozen-hydrated imaging using soft and hard x-rays at resolutions reaching 25 nm and 30 nm respectively [2,3]. This paper will present this recent development in cryogenic (cryo-) XDM with hard x-rays. We have developed non-vacuum cryo-XDM using x-rays at 8 keV with a cryogenic gas-jet environment and imaged a frozen-hydrated bacterium D. radiodurans in natural contrast with a resolution of 30 nm to 50 nm. The recent upgrade of the end station allows 3D data collection in semi-automatic mode to minimize sample degradation during data collection. These developments in cryo-XDM toward high-resolution 3D imaging can provide a method to probe whole-cell architecture in a spatio-temporal investigation of cellular processes.

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[3] E. Lima et al., Phys. Rev. Lett. 103, 198102 (2009).

10th June, 12.00 p.m.

Shape-dependent chemical-induced strains in gold nanocrystals

Prof. Ian Robinson

University College

Shape-dependent chemical-induced strains in gold nanocrystals. Ian Robinson, Moyu Watari, Rachel McKendry, Manuel Vogtli, Gabriel Aeppli, Yeong-Ah Soh, Xiaowen Shi, Gang Xiong and Ross Harder London Centre for Nanotechnology, University College, London

The especially strong bond that forms between sulphur and gold is the basis for numerous self-assembled metal-organic devices. Gold is a noble metal towards almost all environmental species with the exception of sulphydryl-containing species, such as thiols, which readily form monolayer coatings of high stability. The structure of the sulphur-gold interface is remarkably complex. A recent crystallographic study of a monodispersed Au101RS44 gold nanoparticle-thiol complex revealed a crystalline core particle coated with a shell of 1nm thickness with enlarged Au-Au spacings and interpenetration of the thiol ligand species. Far from having a well-defined boundary between the metal and the organic sides of the interface, this unusual complex was found to contain a mixed compound layer as its lowest energy configuration [1]. We report the structure of facetted gold nanocrystals before and after coating with propane thiol, C_3H_7SH, one of the simplest SAM-forming organic molecules. As formed by dewetting a film from a silicon wafer substrate, the shape of our nanocrystals is found to be spherical with {111} facets, as expected from the theory of Equilibrium Crystal Shapes (ECS). The structure of a single 300nm-diameter particle was measured using the powerful technique of Coherent X-ray Diffraction (CXD), which is highly sensitive to the pattern of internal strains within the nanocrystal [2]. Our results show that the strain is profoundly modified by the thiol adsorption. We are able to establish the magnitude of this stress difference using finite element calculations and suggest a model involving preferential reaction on the curved regions of the crystal surface. Figure showing the shape of the crystal and the phase found on the surface of the particle before dosing on a colour scale from -1 (blue) to +1 radian (red). The arrows indicate the {111} directions; the substrate surface normal direction is parallel to the large facet at the top of the figure. The (111) Q-vector used for imaging is on the right hand side. The phase is the projection of the crystal's displacement field onto this direction [2].

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10th June, 12.20 p.m.

Three-Dimensional X-ray Fourier Transform Holography: the Bragg Case

Dr. Virginie Chamard[1], Dr. Julian Stangl[2], Dr. Gerardina Carbone[3], Dr. Ana Diaz[4], Dr. Gang Chen[2], Dr. Claude Alfonso[4], Dr. Cristian Mocuta[5], Dr. Till Harmut Meetzger[6]

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The investigation of strain fields inside nanostructures is a key point for the understanding of physical properties and functionality of materials at the nano-scale. Diffraction techniques are the method of choice for the investigation of strain, as they provide a high resolution for the determination of atomic displacements in crystalline materials. The information on the crystal displacement field is encoded in the phase of the object complex-valued electron density function, but cannot be accessed directly in diffraction experiment [1]. Therefore, great efforts are currently being invested into the "phase retrieval" using coherent radiation. This is achieved by the application of different algorithms whose convergence often depends on the specific case [2]. In any case, 3D strain imaging remains a real challenge for large and/or extended strain fields [3]. Here, a novel approach to determine the 3D structure of nano-scale materials is shown, consisting in the application of x-ray Fourier transform holography in Bragg geometry [4]. The full description of the nano-crystal is directly obtained by a single inverse Fourier transform of the 3D x-ray diffraction intensity hologram, avoiding thereby convergence problems inherent in the lens- less imaging approach based on iterative algorithms. Together with the morphology, Bragg geometry gives access to the 3D atomic displacement field within the crystal. In this presentation, first demonstrations of 3D x-ray Bragg Fourier transform holography using a SiGe holographic nanostructure will be shown. This result opens great possibilities for the investigation of strain fields inside nano-structures in a simple and robust way. This work is funded by the ANR-08-JCJC-0095-01

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Phasing Methods

Chair: *Ian Robinson*

11th June, 09.00 a.m. – Invited Speaker

Imaging Magnetic Structure by Coherent X-ray Diffraction

Prof. Oleg Shpyrko[1], Dr. Ian McNulty[2], Mr. Ashish Tripathi[1], Dr. Sangsoo Kim[2], Mr. Sebastian Dietze[1]

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Scattering with polarized x-rays has contributed immensely to our understanding of magnetism and its behavior in matter. In particular, resonant coherent x-ray diffraction is promising for study of domain structure, transport and dynamics in spin, orbital, and charge-ordered systems ranging from multilayer films to the complex oxides. Transmission x-ray microscopy and x-ray holography are powerful tools for imaging of magnetic structure with synchrotron sources [1,2]; holography experiments are planned for free-electron lasers. These methods traditionally use nanofabricated optics to reach high resolution and circularly polarized light for dichroism contrast. Coherent diffractive imaging can take advantage of linearly polarized light and offers a path to the few-nanometer scale and harder x-rays without precision optics or a phase reference. This talk focuses on recent coherent diffraction experiments on ferrimagnetic GdFe and other vertically anisotropic multilayers. Prospects for imaging the domain structure within these systems by scanning [3] and Fresnel [4] methods are discussed.

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11th June, 09.40 a.m.

A robust coherent imaging approach based on wavefront modulation

Dr. Fucai Zhang[1], Dr. Joan Comamala[2], Dr. Felisa Berenguer[3], Mr. Richard Bean[3], Dr. Cameron Kewish[2], Prof. John Rodenburg, Prof. Ian Robinson[3]

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A novel coherent imaging approach is presented. The approach resolves the two fundamental drawbacks of current coherent diffractive imaging(CDI), namely, the extremely high experimental requirement in data recording and the unreliable and slow convergence for general objects. The approach requires only a single intensity pattern and is able to reconstruct general complex-valued objects uniquely and rapidly. The intensity data are collected with a modulator placed in the path between the sample and the detector. The strong modulation of the modulator greatly reduces the dynamic range requirement of a detector and the brilliance requirement of the radiation source, which in turn alleviates the problem of sample damage. Unlike high quality lenses required in lens-based imaging, there is no strict quality requirement on the modulator. Any fabrication error, if exists, can be easily accounted for in the phasing algorithm. Different modulator design has been tested. The iterative phasing algorithm is adapted to the data recording configuration. It involves propagating wavefield among three planes: the detector plane, the modulator, and a plane (incident plane) that the object wave is known to be spatially finite. In contrast to the conventional CDIs, which usually involves only two planes, the additional beam propagation step between the modulator and the incident plane together with the strong modulation property of the modulator removes those trivial ambiguities in phase problem. As a result, the algorithm converges rapidly even if a rather loose support constraint is used. The approach has been experimentally verified using various samples and different illumination curvature. Within 100 iterations, good reconstruction can be routinely obtained without manually tuning any reconstruction parameters. The approach unifies the lens-imaging and CDI , but disposes their respective limitations. We believe it would turn CDI into a routine technique for applications in material and biological science.

11th June, 10.00 a.m.

Two-dimensional grating-based X-ray phase-contrast imaging with Fourier transform phase retrieval

Dr. Hidenosuke Itoh, Dr. Kentaro Nagai, Dr. Genta Sato, Dr. Kimiaki Yamaguchi, Mr. Takashi Nakamura, Mr. Takeshi Kondoh, Mr. Chidane Ouchi, Dr. Toru Den

Canon Inc.

We demonstrate a single shot two-dimensional grating-based X-ray phase-contrast imaging using a synchrotron radiation source. Grating-based X-ray phase-contrast imaging has been studied with one-dimensional gratings using phase retrieval by fringe scan method, however, multi-shot imaging increases the radiation dose and is not resistant to the movement of the object for medical applications. The Fourier analysis of Moire fringe generated by the gratings was introduced to obtain the two-dimensional differential phase images with a single exposure. The technique has some advantages. This method uniquely determines the phase integrated from the differential phase images, whereas the fringe scan method requires the origin of the integration. The experiments were performed with monochromatic X-rays of 17.5 and 35 keV at BL-20B2 of SPring-8, Japan. A checkerboard designed phase grating for p phase modulation and a lattice-shaped absorption grating were positioned with the 1st Talbot distance. The phase grating was fabricated by a process involving photolithography, deep etching into silicon and, in case of the absorption grating, electroplating with gold. Differential phase image was calculated from the inverse Fourier transformation of a captured 1st Fourier spectrum of the image with Moire fringe. The results show that soft tissues and cartilage of chicken wing sample are clearly seen with differential phase variation in two-dimensional direction. Using this method not only the whole of sample but also only an inner part of the sample can be imaged. In addition, the absorption image can be calculated via the inverse Fourier transform from the 0th Fourier spectrum that is the Fourier transformed from the raw image. The present imaging method shows that we can obtain both two-dimensional phase differential image and the absorption image of any part of samples with a single exposure.

11th June, 10.20 a.m.

Development of a Novel Holography Technique for X-ray Coherent Diffractive Imaging

Manuel Guizar-Sicairos, James Fienup

University of Rochester

Application of holography to x-ray diffractive imaging offers a significant computational advantage over iterative transform phase retrieval algorithms (ITAs) that rely on a support constraint [1,2]. X-ray Fourier transform holography (FTH) offers a simple, closed-form, and fast reconstruction algorithm that requires no a priori information and is robust to noise and measurement errors [3,4]. However in many cases the resolution in the reconstruction is limited by the capability to produce a small coherent point source next to the object. We have introduced a method for off-axis holography for which the holographic reference wave is provided by a boundary wave emerging from a sharp feature on an extended reference structure. Holography with extended reference by autocorrelation linear differential operation (HERALDO) [5] allows the use of a wide class of extended references, beyond the pinhole of FTH and the rectangular structure proposed earlier [6], including thin slits, nanowires, crossed-wires [7], corners and tips. Choice of structures that can be naturally grown to be sharp can lead to improved resolution over FTH. This technique has a simple closed-form reconstruction algorithm that can be performed using parameters that are easily estimated from the measured diffraction data. The noise and artifact robustness, improved resolution and versatility of this technique has been recently demonstrated at optical wavelengths [8,9], x-ray CDI experiments [7,10], and through reconstructions from single-shot data from a table-top source [11].

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FEL Based Imaging

Chair: *Janos Kirz*

11th June, 11.00 a.m. – Invited Speaker

Single Shot 3D Imaging of Sparse System using Compressed Sensing

Filipe Maia

Biomedical Center, Dept. of Cell and Mol. Biol., Uppsala Universitet

Single pulse diffractive imaging allows, in principle, to obtain 3 dimensional images of perfectly reproducible samples. The method involves collecting multiple diffraction patterns of identical samples, assembling them into a 3D Fourier volume and then phasing the resulting volume. But there is a vast group of important samples for which it is very hard or impossible to obtain identical copies. In this case we can only obtain one single shell from the 3D Fourier volume. If we then only use the low angle data we can obtain a 2D quasi-tomographic image of the sample. In this talk I will discuss the possibility of obtaining full 3D images from a single shot in the case of sparse samples. Powerful optimization tools provided by the booming mathematical field of compressed sensing make it possible to fully recover the 3D Fourier volume, starting from a single Fourier shell, opening the way for 3D imaging of non reproducible simple sparse systems.

11th June, 11.40 a.m.

Determination of biomolecular structures using fourth-generation X-ray sources

Dr. Harry Quiney, Mr. Evan Curwood, Prof. Keith Nugent

The University of Melbourne

Proposals to harness the brilliance of X-ray free-electron laser sources to determine the structures of nanocrystals or individual biomolecules [1,2] from diffraction have recognized that electrodynamical processes play a critical role in the analysis [3,4]. Even if the pulse incident on the molecule is short enough that the nuclear framework is not disrupted during the collection of scattered photons, the electron density evolves rapidly throughout the interaction. The dynamical character of the interaction invalidates the fundamental paradigm of X-ray crystallography, in which a ground-state electron density is associated with a properly-sampled diffraction pattern through a single Fourier transform relationship. We show that a consequence of these electrodynamical processes is that X-ray diffraction data collected under conditions that have been proposed as suitable for molecular imaging exhibit characteristic signatures of a partially-coherent source [5], even if the illumination incident on the scattering target possesses full spatial and temporal coherence [6,7]. Assuming that a three-dimensional scattering data set has been constructed from many randomly-orientated two-dimensional projections [8], under the condition that each illuminating pulse is of 5 fs duration and consists of 10^(12) 5 keV photons, we have devised a computational scheme to reconstruct the molecular structure of biomolecules that incorporates the effects of electronic damage. Molecular structures are obtained without recourse to representations of their corresponding electron densities or any of the associated molecular modelling that accompanies conventional approaches to protein crystallography. The scheme may also be used to characterize the extent of electronic damage when applied to molecular targets of known structure, providing an experimental calibration of the approach and a direct experimental probe of multi-photon excitation processes induced by an XFEL source. The implementation of the scheme is illustrated by simulated molecular structure determinations of the membrane protein bacteriorhodopsin under interaction conditions typical of those that have been proposed for diffraction experiments using XFEL sources.

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11th June, 12.00 p.m.

An instrument for nanocrystal diffraction and imaging at the LCLS

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Since 1999, coherent x-ray imaging has progressed from initial demonstration to a foundational tool for important aspects of the science case for fourth generation X-ray sources. In particular, X-ray free electron lasers (XFEL) promise never before seen levels of high-brightness photon flux, which enables an entirely new class of experiments to be performed. The extremely high peak power of an XFEL beam provides access to very-short-time-scale imaging and may allow structure determination of radiation-susceptible samples before significant damage occurs. We will present a purpose-built instrument designed to take full advantage of the unique XFEL beam provided by the Linac Coherent Light Source (LCLS), which will become the first hard XFEL user facility in the Fall of 2010. The coherent X-ray imaging instrument (CXI) will support both coherent imaging and crystal diffraction experiments, with an emphasis toward structure determination from micron-sized objects at resolution of order the X-ray wavelength. The instrument includes a suite of optics and diagnostics, a flexible sample chamber, and a novel large area pixel array detector--all of which will be described in detail.

11th June, 12.20 p.m.

Ultrafast Resonant Magnetic Scattering at the Free-Electron Laser FLASH

Mr. Bastian Pfau[1], Mr. Christian Günther[2], Dr. Christian Gutt[3], Dr. Simone Streit-Nierobisch[3], Dr. William Schlotter[4], Prof. Jan Lüning[5], Dr. Gerhard Grübel[3], Prof. Stefan Eisebitt[1]

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The fundamental understanding of strongly out-of-equilibrium magnetization dynamics such as in ultrafast demagnetization is an outstanding challenge in modern physics with potential applications in spintronics and magnetic data storage. The elementary spin dynamics and their coupling to the electronic system is intrinsically acting on a sub-picosecond timescale and can be very selectively studied by x-rays. FEL-based x-ray light sources are able to deliver highly intense femtosecond x-ray pulses that are an ideal probe to study fundamentals in magnetization dynamics. Here we report on the first ultra-fast resonant magnetic scattering experiments carried out at the FEL facility FLASH, Hamburg. The measurements were performed mainly at the Co M-egde (at 20.9 nm x-ray wavelength), but also at Co L3-edge (1.6 nm) using FLASH lasing in the fifth harmonic. We present magnetic small-angle scattering (SAXS) patterns of magnetic labyrinth domains in Co/Pt multilayers recorded within single 20 fs long x-ray pulses. The experiments were run either in destructive mode, i.e. the sample was destroyed after a single FEL pulse, or non-destructive mode. We discuss the damage thresholds and FEL induced changes as evident from the SAXS signal. The same x-ray scattering probe with a preceding 120 fs optical pump was used for IR-pump X-ray-probe experiments. We can clearly detect the induced ultrafast demagnetization via changes in the recorded SAXS spectra. In addition to the ultrafast reduction in overall magnetization after the pump, we detect an increase of the domain size on the same timescale. The time resolution in pump-probe experiments using an optical pump is limited by the duration of the pump pulse and the time jitter between the optical laser and the FEL source. In order to overcome this limitation, we performed x-ray-pump x-ray-probe experiments where the pump and the probe pulse were generated from a single FEL pulse using a split and delay approach. These experiments exploit the high degree of coherence of the FEL radiation and the magnetization dynamics is analyzed via the speckle statistics in the superimposed resonant SAXS patterns. Based on this work, we present an outlook for ultrafast magnetic imaging using Fourier transform holography at the existing FEL sources.

11th June, 12.40 p.m.

Dense Xenon Nanoplasmas in Intense Laser Fields

Dr. Thomas Bornath[1], Dr. Paul Hilse[2], Max Moll[2], Prof. Manfred Schlanges[2]

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[2] Ernst Moritz Arndt University Greifswald

The interaction of intense laser fields with xenon and silver clusters is investigated using the nanoplasma model. An effective tool to control the plasma dynamics is pulse shaping, i.e., a modulation of phase and amplitude of the laser pulse. In particular, the yield of highly charged ions can be controlled. For an understanding of the underlying physical processes in the dynamics of laser- cluster interaction, a theoretical description using a genetic algorithm and basing on the relatively simple nanoplasma model seems to be promising. In the present approach, the time evolution of the laser intensity has been parametrized. The parameters where optimized with a genetic algorithm to get, e.g, a maximal yield of a specific ion species.

Poster Presentations

Poster Number: 1

Soft glasses studied by X-ray photon correlation spectroscopy

Dr. Birgit Fischer[1], Dr. Christian Gutt[1], Prof. Joachim Wagner[2], Fabian Westermeier[1], Dr. Gerhard Grübel[1]

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The understanding of the dramatic slowing down and non-exponential relaxations in glasses and dense colloidal suspensions is one of the most challenging problems in condensed matter physics. Recently, the concept of "heterogeneous dynamics" has attracted much attention as it is considered a key ingredient for understanding the drastic slowing down at the glass transition without significant changes in the structure. Here, we will present the structure and dynamics of three different charged colloidal systems with different volume concentration studied with coherent small angle X-ray scattering methods. The static structure factor indicates that the degree of ordering depends on both the electrostatic interactions and the volume fraction. In all cases the dynamic structure factors show a compressed exponential form. The Q-dependence of the relaxation time hints towards ballistic motion of the colloidal particles in the glassy state. For the sample with the highest volume fraction we observe an influence of the static structure factor on the relaxation rate of the particles indicating a caging effect also for the ballistic type of motion.

Poster Number: 2

Anisotropic diffusion of ellipsoidal particles in supercooled suspensions studied by X-Ray photon correlation spectroscopy

Dr. Louisa Dahbi[1], Prof. Joachim Wagner[2], Christian Gutt[1], Dr. Gerhard Grübel[1]

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In colloidal suspensions, the motion of particles is governed by their size and shape along with the solvent viscosity and temperature. In general, both translational and rotational degrees of freedom contribute to the overall particle dynamics with both motions coupled in the case of anisotropic particles [1]. By means of X-ray photon correlation spectroscopy [2,3], we explore the dynamics as well as the dynamical heterogeneities of ellipsoidal particles in suspension (hematite a-Fe_2O_3, fig. a) when their dynamics is slowed down by decreasing the temperature of the solvent close to the glassy state. Two kinds of experiments were performed. In the first type of experiment, the single experimental parameter was the temperature while in the second type of experiment a constant magnetic field was applied as additional parameter to hinder the rotational motion of the particles in one direction. We will show how the dynamics of the particles is changed when either the temperature or the rotational dynamics is quenched in one direction by applying a magnetic field. Finally, the role of the aspect ratio of the particles for the dynamics will be discussed. a) Anisotropic a-Fe_2O_3 (hematite) cigar shaped particles b) X-ray photon correlation spectroscopy principle: $g2(q,t) = \langle I(q,t)I(q,t+t) \rangle / \langle I(q,t) \rangle 2$ c) SAXS pattern (the particles are aligned along the vertical axis using a magnetic field of 120 mT) d) Corresponding correlation function in the vertical and horizontal direction, the full and open circles represent the correlation function in the vertical and horizontal direction respectively (insert: two times correlation function, showing the dynamical heterogeneities).

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Poster Number: 3

Measurements of the dynamic susceptibility of colloidal suspensions using coherent X-rays

Mr. Heiko Conrad, Dr. Louisa Dahbi, Dr. Birgit Fischer, Dr. Christian Gutt, Dr. Gerhard Grübel

Hasylab at Desy

A coherent X-ray beam scattered by a quasistatic disordered sample generates a speckle pattern which reflects the exact spatial arrangement of the particles. By calculating the time autocorrelation function the characteristic time scale of the dynamics can be extracted from the speckle pattern. This technique provides information on the dynamics of soft condensed matter systems. In this context colloidal particle are often used as tracer to detect the dynamics in molecular glass former. We studied silica particles with a size of about 100 nm in glass forming liquids using X-ray photon correlation spectroscopy (XPCS) coupled with small-angle X-ray scattering (SAXS) to investigate the glass transition phenomena. In recent years, numerous works have focused on the role of dynamic heterogeneities as underlying reason for the dramatic increase of the viscosity when approaching the glass transition temperature. We present our latest data applying the four-point density correlator G4 as a function of temperature and wave vector transfers. Theory predicts notable differences in the behavior of the corresponding dynamic four-point susceptibility function $\chi 4$ for the usual glass formation models. The combination of the information on dynamic heterogeneities along with time dependent local symmetries opens a new route to understand the glass transition.

Poster Number: 4

Non-stationary dynamics and dynamical heterogeneity in polymer gels by XPCS

Dr. Orsolya Czakkel, Dr. Anders Madsen

ESRF

Polymer aerogels constitute an important class of new carbon forms due to the versatility of their pore structure and their surface properties. Their applications are numerous, ranging from electrical capacitances, batteries, catalyst supports, to toxic gas protection devices [1]. Thanks to the sol-gel preparation method, heteroatoms (e.g metals) can easily be introduced and used as catalysts during the polymerization, which opens new fields of application for these materials. The polymerization reaction is of fundamental interest and a deeper understanding of this process is the key factor to achieve a successful doping. Multi-speckle (2D) X-ray photon correlation spectroscopy (XPCS) is a new powerful method to characterize the q-dependence of non-stationary dynamics during the sol-gel transition as well as investigating stress-induced complex relaxation process in the aerogel state. Here we show first results obtained on polymer gel systems using 2D XPCS with emphasis on the dynamical aging process and its q dependence, as well as the observed dynamical heterogeneity [2].

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Poster Number: 5

Application of Conjugate Gradient and Quasi-Newton Algorithms to Pytchography

Mr. Ashish Tripathi

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Learning to control emergent magnetic properties such as colossal magnetoresistance and phase separation is crucial for developing future spin-based data storage and computational technologies. Probes with the ability to map magnetically interacting materials beneath surfaces on the nanometer scale, ultimately on ultrafast time scales, would greatly enhance our understanding of these systems. Scanning Coherent X-ray Diffraction Microscopy (SXDM) is a promising new technique [1,2] for imaging magnetic nanostructure with potentially wavelength-limited resolution that can probe beneath surfaces. The essence of this technique is that, rather than using optics to image the nanostructure, we record a series of coherent diffraction patterns as the sample is scanned, then algorithmically invert them using known constraints on the sample (real space) and on the diffraction measurements (reciprocal space) to arrive at the sample structure. Although preliminary experimental results using this technique are promising [3], existing SXDM algorithms depend on a steepest descent gradient and are thus prone to certain weaknesses: stagnation and slow convergence in valleys and other relatively flat areas in the error metric space. In other words, these methods can fail with relatively weak constraints to guide convergence. Conjugate gradient and quasi-Newton algorithms are not as prone to this behaviour. Here, we explore improved convergence properties using these algorithms in simulation with realistic experimental limitations such as missing data regions and noisy diffraction data.

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Poster Number: 6

Bragg Geometry Ptychography

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Ptychography is a coherent diffractive imaging technique which solves the phase problem by using the redundancy in a set of diffraction patterns collected from overlapping regions of a sample. The method is ideal for imaging extended non-periodic structures where the support constraint required by HIO methods cannot easily be defined. At X-ray wavelengths samples including Fresnel zoneplates and biological cells have been imaged using Ptychography in transmission geometry. Recent advances in the Ptychography phase retrieval algorithm have allowed for the simultaneous reconstruction of the object and illuminating wavefront, increasing the application potential of the technique. Coherent X-ray Diffraction in Bragg geometry has been successful for imaging isolated nanocrystals, revealing information about their growth and strain. We have extended Ptychography into Bragg Geometry to image extended structures using individual Bragg peaks. Speckle distribution in the Bragg peaks contains information on the relative position of the scattering centres in the sample. In contrast to transmission geometry Bragg Ptychography reconstructs a dark field image of the ordering phenomenon responsible for the speckle distribution in a given scattering peak and can therefore selectively image structures where other ordering phenomena or materials are present. This selectivity gives access to a wide range of scientifically important problems from surface structures to protein filament ordering in biological tissue to charge and magnetically ordered domains where transmission imaging is not possible in general. Ptychography has the additional advantage of avoiding the mechanical sectioning which can affect the structure being imaged. A proof of principle of the technique is presented by the imaging of a deliberately designed test structure. Our sample is an array of randomly distributed but aligned gold 'ladder' motifs on a silicon nitride membrane fabricated by e-beam lithography at the Paul Scherrer Institute. The motif is designed to have Bragg peaks accessible by our CCD detector in a forward scattering geometry. A series of Ptychographic data sets were taken at the cSAXS beamline of the Swiss Light Source under a range of conditions. We have shown it is possible to reconstruct both the sample structure and illuminating wavefront using only the information contained in the Bragg peaks of the sample. The results are consistent with our simulated tests on the same design. The future application of the method is discussed.

Poster Number: 7

Hard x-ray nanobeam characterization by coherent diffraction microscopy

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We have carried out a ptychographic scanning coherent diffraction imaging experiment on a test object in order to characterize the hard x-ray nanobeam in a scanning x-ray microscope. In addition to a high resolution image of the test object, a detailed quantitative picture of the complex wave field in the nanofocus in obtained with high spatial resolution and dynamic range. Both are the result of high statistics due to the large number of diffraction patterns. The method yields a complete description of the focus, is robust against inaccuracies in sample positioning, and requires no particular shape or prior knowledge of the test object.

Poster Number: 8

Some Improvements in the Ptychography Iterative Engine

Dr. Pierre Godard[1], Dr. Virginie Chamard[2]

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The detailed knowledge of the internal structure on the nanoscale is a fundamental prerequisite to understand and monitor the physical properties of nanostructures. Hard x-rays are often applied as a probe. Due to the high sensitivity of x-rays to the atomic positions, Bragg x-ray diffraction is particularly relevant to study strain field in nano-crystals. However the impossibility to directly image the strain field is a strong limitation to the method. Recently developed lens-less x-ray microscopy techniques provide an elegant solution to the phase problem. These imaging techniques are based on the digital retrieval of the phase from the object's coherently diffracted intensity patterns. The strain field is introduced in a complex-valued effective electron density function, where the phase is the projection of the displacement field onto the Bragg vector. The retrieved quantity is the product of the illumination function with the electron density. Therefore, any phase shift already present in the illumination function will appear as an artefact in the displacement field. In this context, the recently demonstrated ptychographic approach is of particular interest to study strain field in a nanocrystal as it allows for the imaging of both functions, separately [1]. We will present some new developments of the Ptychography Iterative Engine (PIE): (1) a usual limit of the ptychography approach is the presence of periodic defects in the retrieved object function [2]. It results from a local defect in the retrieved illumination function, which is reflected back in the guessed object, since the exit field, in the far-field approximation, is the product of the two functions. Due to the periodicity of the translation of the illumination onto the sample, these defects appear periodically. Using a reciprocal space approach, we are able to correct this problem. (2) The PIE engine is highly sensitive to the initial estimate. Based on the approach developed by Chen and co-workers [3], we have implemented a genetic method in the iterative process. These new developments are successfully numerically tested in the case of strained crystals. This work is funded by the ANR-08-JCJC-0095-01.

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Poster Number: 9

Analysis of Femtosecond X-ray Laser Nanocrystal Diffraction Patterns

Thomas White[1], Andrew Martin[1], Francesco Stellato[1], Karol Nass[1], Anton Barty[1], Andrew Aquila[1], Henry Chapman[1], Richard Kirian[2], Petra Fromme[2], Mark Hunter[2], Uwe Weierstall[2], Bruce Doak[2], John Spence[2], Lukas Lomb[3], Thomas Barends[3], Robert L. Schoeman[3], Daniel Rolles[3], Loutz Foucar[3], Ilme Schlichting[3], James Holton[4], CAMP collaboration[5]

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Fourth generation light sources – free-electron lasers (FEL) - are opening new possibilities for the X-ray diffraction imaging, because the high brilliance and the short time duration of their pulses allow the study of small crystals that are not accessible for standard crystallography. FEL radiation indeed allows individual diffraction patterns to be recorded before significant damage to the specimen occurs [1,2]. The point is that each pulse destroys any specimen in a very short time, and therefore intensities from many thousands of individual diffraction patterns have to be summed up in order to obtain integrated Bragg intensities [3]. To achieve this requires, amongst many other things, high-throughput processing and indexing of patterns in a highly automated manner. Here we describe the application of such indexing techniques to the experimental data acquired on the membrane protein Photosystem I at the Linac Coherent Light Source (LCLS). Photosystem I crystals smaller than 2 micron are injected, using a continuous liquid jet, onto the pulsed X-ray beam. Millions of diffraction patterns are recorded at the repetition rate of 30 Hz with pnCCD detectors [4]. The indexing algorithm is then applied to the data, allowing a successful indexing of tens of thousands patterns [5]. The analysis of the indexed patterns allows the study of the effects of pulse duration and fluence. We finally show how it is possible to reconstruct the image of entire Photosystem I crystals by applying iterative phase retrieval algorithms [6].

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Poster Number: 10

Analytical reconstruction of images obtained using a URA aperture in X-ray holography

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It has recently been shown by Marchesini et al. that Uniformly Redundant Arrays (URAs) can be used as reference objects in X-ray holography. We have investigated the possibilities and limitations of analytical, i.e. non-iterative, reconstruction of images using a scheme where an image of the URA itself is part of the recorded hologram. Even though we find that the ability to nano-structure the URA aperture limits the quality of analytical reconstruction, we show that it is possible to perform the image analysis online and very quickly utilizing the extra recorded information. This is of significant value in, for example single-shot imaging, as the ability to perform data analysis during the experimental run is often paramount to the success of such measurements.

Poster Number: 11

Coherent Diffraction Imaging of Atomic Clusters with Free-Electron Lasers

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The problem of radiation damage becomes significant in high-resolution coherent diffraction imaging (CDI) with intense free electron lasers (FELs), especially for biological samples consisting of light atoms. Additional difficulty of low signal-to-noise ratio (SNR) in diffracted patterns limits experimental study of this problem within CDI of single bio-particles. Atomic clusters, as a simple model of molecules, are utilized as imaging objects to reveal dynamics of the radiation damage. In this work, we present analysis of the pattern data from the first imaging experiments of atomic clusters at FLASH. As a primary step in the study of radiation damage, we focus on the reliable reconstruction of the cluster objects.

Poster Number: 12

Coherent Diffractive Imaging of Fixed Target Samples at FLASH

Dr. Adrian Mancuso[1], Dr. Andreas Schropp[2], Mr. Bernd Reime[1], Dr. L. M. Stadler[1], Mr. Andrej Singer[1], Mr. Jochanes Gulden[1], Dr. S. Streit-Nierobisch[1], Dr. Christian Gutt[1], Dr. G. Grübel[1], Dr. J. Feldhaus[1], Dr. F. Staier[3], Dr. Ruth Barth[3], Dr. Axel Rosenhahn[3], Prof. M. Grunze[3], Mr. T. Nisius[4], Dr. T. Wilhein[4], Mr. D. Stickler[5], Dr. H. Stillrich[5], Dr. R. Frömter[5], Prof. H. Oepen[5], Dr. M. Martins[5], Mr. B. Pfau[6],Mr. C. M. Günther[6], R. Könnecke[6], Prof. S. Eisebitt[7], Dr. M. E. Pettit[8], C. Christophis[3],Dr. B. Faatz[1], Dr. N. Guerassimova[1], Dr. K. Honkavaara[1], V. Kocharyan[1], R. Treusch[1], E. Saldin[1], S. Schreiber[1], E. A. Schneidermiller[1], M. V. Yurkov[1], Prof. E. Weckert[1], Mrs. I. A. Vartanyants[1]

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The Free-electron LASer in Hamburg (FLASH) at DESY was the first operating free-electron laser (FEL) in the XUV energy range [1]. An overview of recent Coherent X-ray Diffractive Imaging (CXDI) experiments on periodic [2] and non-periodic biological samples [3] at FLASH will be presented. The first example in this presentation is a CXDI reconstruction of a two-dimensional (2D) finite crystal structure, measured with a single pulse train of FLASH radiation at 7.97 nm wavelength [2]. This measurement demonstrates an advance on traditional CXDI techniques by applying it to a periodic structure of finite extent. This method introduces the possibility of imaging the class of specimens which readily form 2D, but not three-dimensional crystals. We show that the structure is reconstructed to the detected resolution, given an adequate signal to noise ratio. We have also employed CXDI using FLASH in a non-destructive regime to compare images of a biological sample measured using different, single, femtosecond pulses of FEL radiation [3]. We have demonstrated that images reconstructed from statistically different FEL pulses are quantitatively similar up to the measured resolution. This result is particularly important for the success of the single molecule imaging approach [4], which utilizes different, single FEL pulses to image identical samples. Furthermore, for the first time, we demonstrate CXDI, in-line holography and Fourier Transform Holography (FTH) of the same unicellular marine organism using an FEL and present diffraction data collected using the third harmonic of FLASH, reaching into the water window. We provide results for the resolution of the CXDI images as a function of pulse intensity, and compare this with the resolutions achieved with in-line holography and FTH.

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Poster Number: 13

Coherent Diffractive Imaging of Two and Three-Dimensional Membrane Protein Crystals using XFELs

Ms. Rebecca Ryan, Prof. Keith Nugent, Dr. Harry Quine

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The potential for imaging biomolecules using fourth generation XFEL sources is now being explored with the commisioning of beamline experiments having begun at the LCLS (Stanford). These experiments will employ the use of coherent X-ray diffractive imaging techniques by collecting snapshot diffraction patterns in a time regime that avoids nuclear damage in biomolecules. The opportunity to perform imaging of single biomolecules (such as membrane proteins) is present. Some membrane proteins form single two-dimensional crystals and submicron single three-dimensional crystals. Diffraction data collected from periodic samples (such as these small membrane protein crystals) will provide both an amplified intensity measurement and additional a priori constraints(the periodicity of the sample) that will benefit image reconstruction. We have simulated the diffractions produced using XFEL radiation for two-dimensional and three-dimensional submicron crystals of the membrane proteins lysozyme, potassium channels and bacteriorhodopsin for upcoming experiments. We seek to perform appropriate phase-retrieval on this data that will lead to high
resolution solutions to membrane-protein structures. Neutze et al. (1) first suggested the use of XFELs for biomolecular imaging since the timescale of X-ray pulses irradiating membrane-protein samples (~5-50 femtoseconds) is such that nuclear damage may be avoided. Further consideration has also been paid to damage to the electronic structure of such biomolecules under intense radiation (2). Coherent Diffractive Imaging (CDI) is an imaging technique that has been developed to image objects that are non-crystalline (3)(4) with X-rays. The object structure is reconstructed from the diffraction data image using phase-retrieval algorithms (5)(6). It has been demonstrated that appropriate real-space constraints (information about the sample object such as its size) or implementation of knowledge about the wavefield in phase-retrieval algorithms improves the reconstruction of the sample (7)(8). The collection of diffraction data and analysis from single molecules and small two-dimensional membrane protein crystals using XFEL pulses has been considered (9)(10)(11). We have performed diffraction simulations for submicron membrane protein crystals incorporating the X-ray intensities supplied at LCLS, Stanford. We seek to develop implement CDI techniques for resolving high resolution information from this data for experiments to be performed in the near future.

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Poster Number: 14

Towards time-resolved imaging at x-ray free-electron lasers

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To record a „molecular movie“ with atomic spatial resolution on the femtosecond timescale set by atomic motion can be considered as the ultimate goal of dynamic microscopic imaging. Free electron x-ray lasers with their (sub-)nanometer wavelength, femtosecond pulse duration and high brilliance fuel the hope that this may become possible. Single-shot still pictures with nanometer resolution during femtosecond exposures have already been demonstrated [1]. The next step towards time-resolved movies is to generate an image-series during sample evolution on the pico-, and nanosecond time scale. In this ultrashort regime imaging approaches have to be modified to take technical obstacles, like the repetition rate of FEL or the readout time of detectors, into consideration. Here, we demonstrate two imaging approaches capable of probing a specimen multiple times at adjustable time delays. In FTH, multiplexing [2,3] is a way to generate a multitude of pictures for a series of samples with the same pulse of light simultaneously. Using sample multiplexing we demonstrate parallel single-shot Fourier transform holography over an extended field of view with eight samples obtaining clear reconstruction from every object. The idea is to include an angle between a laser pump and the x-ray probe as discussed in [3]. Assuming identical behavior for the investigated specimens the resulting time ramp allows to image the samples dynamic response at several time delays, simultaneously. An experiment allowing to image one sample twice with a femtosecond time delay requires a more sophisticated setup. An autocorrelator [4] acting as efficient soft-x-ray beam splitter allows to perform a Fourier transform holography experiment in a cross-beam setup. The two beams are aligned in such way that each of them is fully illuminating the object, but only partly the multiplexing reference arrangement [5]. The two resulting holograms with inherent time difference are recorded superimposed on a CCD camera. During the reconstruction process the reference-object cross-correlations, which present individual images of the object, are separated in space. As a result, an assignment of each of these images to the corresponding probe-beam and therefore to their different recording time is possible. Due to this disentanglement our concept overcomes the readout time limitations of 2D area detectors.

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[4] R. Mitzner et al., Opt. Express, 16, 19909 (2008)
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Poster Number: 15

Study of a damage amelioration scheme for high intensity x-ray measurements of a single biomolecule

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The intense illumination expected from an X-ray free electron laser (XFEL) causes dynamical changes to the electronic structure of a single biomolecule. Studies of a scheme to overcome this effect on the coherent diffractive imaging (CDI) measurement are presented. The study focuses on simulation of the coherent diffracted intensity of a single membrane protein, bacteriorhodopsin. It is shown that the effect of the damage on the measured intensity may be modeled as a partially-coherent optical process, and a successful reconstruction of the molecular structure may be obtained directly.

The reconstruction of the structure of biomolecules to atomic resolution requires sufficient signal scattered to a high angle, facilitating the need for illumination from ever more brilliant sources, such as the new XFELs [1]. Exposure from such high fields creates an evolving electronic structure, which degrades the far-field intensity measurement [2]; the measurement is preferentially degraded in regions of high angle leading to a reduction in reconstructed resolution . This requires modeling the diffracted intensity as a partially-coherent optical process, regardless of the coherence of the incident beam. The scheme expands the diffracted intensity into structural and dynamical components, calculated assuming knowledge of the primary structure of the molecule, and the photo-absorption cross-section and Auger recombination rates. The dynamical components may be used to preferentially scale the measurement to ameliorate the damage prior to input into a standard Gerchberg-Saxton-Feinup iterative phasing algorithm to reconstruct the undamaged electron density. A further addition to the scheme allow for the reconstruction of the structural information directly. Simulated reconstructions made using these schemes, of both the electron density and structural information of the biomolecule bacteriorhodopsin are presented.

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[2] Neutze et al. (2000) Nature 406, 752-757

Poster Number: 16

Clusters in intense XUV pulses: Ionization heating and time-resolved imaging of cluster space-charge potentials

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The excitation mechanisms of clusters exposed to intense laser fields in the XUV and soft x-ray domain strongly differ from the response behaviour in the near-infrared wavelength range. Whereas the heating of delocalized electrons in the nanoplasma is the dominant energy capture mechanism in optical fields, energy absorption due to the excitation of localized electrons, i.e. by the inner ionization processes itself, becomes increasingly important at high photon energy. Further, the formation of a nanoplasma is substantially delayed because of direct electron excitation into the continuum. The resulting signatures in electron energy spectra can be described by a multi-step ionization scheme and subsequent thermal electron evaporation from the nanoplasma. Corresponding results from molecular dynamics simulations will be presented. We further propose a non-optical scheme to directly measure the cluster explosion dynamics and the evolution of the nanoplasma by tracing the cluster space-charge potential in a two colour pump-probe experiment. Numerical results on this time-resolved potential streaking will be discussed and it will be shown that our approach offers a promising new route to access ultrafast ionization dynamics in finite samples. The direct access to the cluster space-charge potential is of high relevance for assisting x-ray single shot diffraction measurements because of the possibility to extract spectral properties of the nanoplasma.

Poster Number: 17

Single and multi-electron emission from clusters with FLASH

Prof. Karl-heinz Meiwes-Broer[1], Dr. Volkmar Senz[1], Prof. Thomas Fennel[1], Jens Bahn[1], Patrice Oelßner[1], Dr. Josef Tiggesbäumker[1], Dr. Christoph Bostedt[2], Prof. Thomas Möller[2]

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Subject is the photoemission from metal and rare gas clusters with FLASH. Interesting many-electron and correlation effects are seen in the experiments as well as in the corresponding theoretical work.
V. Senz, Th. Fennel, J. Bahn, P. Oelsner, J. Tiggesbaumker, C. Bostedt*, Th. Moller*, K.-H. Meiwes-Broer University of Rostock, 18051 Rostock, Germany *Technical University Berlin, 10623 Berlin, Germany Metal clusters serve as model systems to study basic problems of electronic correlation. [1] Free mass-selected metal cluster anions have been prepared with the number of atoms exactly known and have been studied with core-level photoelectron spectroscopy. VUV light from the free-electron laser FLASH ionizes shallow core levels from the negatively charged clusters, thus transiently leading to core-ionized neutral systems. The instantaneous shielding of the core-hole affects the measured binding energy of the departing photoelectron. From the strong deviation from expectations of the metallic droplet and jellium models we conclude on reduced electronic shielding once the cluster size falls below about 20 atoms. [2] This suggests a metal-to-nonmetal transition, in agreement with previous LDA calculations. Moreover, at given photon energy ranges photoemission can be completely dominated by secondary effects, e.g. Auger emission. Strong field photoexcitation with focussed FEL radiation may lead to interesting many-electron effects. This has theoretically and experimentally been studied with rare gas clusters. [3] As a result, after initial ionization and build-up of strong confining potential, further electron emission is hindered; instead we observe a transition to plasma heating.

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[2] Senz et al., Phys. Rev. Lett. 102, 138303 (2009)
[3] Bostedt et al., Phys. Rev. Lett. 100:133401, 2008

Poster Number: 18

Biological Tissues Imaged by Dark Field Coherent X-ray Scanning Phase Modulator Methods: limitations and perspectives

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The applications of Coherent X-ray Diffraction (CXD) methods to the dark field imaging of biological specimens are still limited despite of the possibilities that the technique can offer. CXD reconstructed images will show with enhanced contrast the distribution of a particular component within a complex sample, for instance the distribution of a given filamentous protein inside a tissue. This is of particular interest for the imaging of collagen distributions in complex hierarchical tissues such as tendon or bone. However, there are several difficulties to address: the effects of radiation damage, the limited scattering power of the samples (which demands high dynamic range of the detectors), the thicknesses of the sample, in the order of some hundreds of microns or even millimetres, which induce several phase wraps in the diffracted waves, increasing the difficulty of the CXD reconstruction; and the poor precision of the probe positions on the sample, which makes difficult the use of conventional ptychographic algorithms. The use of a known phase modulator scanned downstream the sample can help to overcome some of these difficulties. The known phase distribution of the phase adds additional constraints to the sample phase recovery process. Also, it homogenises the diffracted intensity, reducing the demands in terms of detector dynamic range. In this communication, we present our results regarding the feasibility of this technique to be used for the dark field imaging of biological tissues. Coherent X-ray diffraction patterns from freshly dissected rat tail tendon samples were collected at the cSAXS beamline in Swiss Light Source using a specially designed Au plate as phase modulator downstream the sample. The plate consisted in an ordered array of motifs mimicking the collagen fibrils distribution, shape and size within the tendon sample; therefore its Bragg diffraction peaks superimposed the ones from the biological sample. The phase shift induced by the plate was chosen to match also the expected phase shift from the tendon in order to balance the intensity contributions to the diffraction pattern of both sample and plate. Exposures of 30 sec were taken with a 10 micron beam during a scan of the phase plate located a few millimetres downstream the sample. The resulting diffraction patterns were recorded with a 20 micron pixel CCD detector. We expected that the total intensity recorded on the detector would correspond to the diffracted intensity from the sample (weak as expected from a biological soft tissue), plus the one from the plate, plus an interference term that would be particularly relevant as it will help in the reconstruction of the sample giving extra constraints to the possible values for the object phases. However, in our results these interference effects are not clearly visible, implying that the use of a phase modulator for improving the reconstruction process has some experimental limitations. The implications of this fact will be discussed.

Poster Number: 19

Analysis of perturbative phase retrieval for single-distance radiogram

Mr. Julian Moosmann, Mr. Ralf Hofmann

KIT/ANKA

We analyse the results of a perturbative method, see talk by Ralf Hofmann, to retrieve contact-plane phase contrast from single-distance intensity contrast applied to the Shepp-Logan phantom both in 2D real and 1D Fourier space (line-cut through contact-plane phase contrast). For phase retrieval according to this method next-to-leading and next-to-next-to-leading order corrections are considered. To analyse these corrections, a particular regularization for the inversion of the 2D Laplacian and various error measures are introduced. Within a rather broad window of distances z we find a considerable improvement of the lowest-order result in real space (~35 %). The spectral analysis indicates a significantly improved retrieval of the Fourier weight of 1D cuts through the contact-plane phase contrast within particular frequency ranges. We hope to be able to present an analysis of real data as well.

Poster Number: 20

Foundations of perturbative phase retrieval for single-distance radiogram

Mr. Ralf Hofmann, Mr. Julian Moosmann

KIT/ANKA

For pure phase objects we device a perturbative series in object-detector distance z for the retrieval of a 2D phase map in the contact plane (z=0) out of a single-distance 2D propagation-induced intensity contrast measured at z>0. Here we consider a monochromatic, coherent, and parallel incident X-ray beam. Both intensity and phase contrast at z>0 are expanded into a power series in z with coefficients determined by the real and imaginary (TIE) part of the paraxial wave equation. For the phase contrast at z=0 this yields a 2D nonlinear partial differential equation expressing the Laplacian in terms of measured intensity contrast and a polynomial in □ invoking transverse derivatives, quartic and higher power counting in z, this polynomial is evaluated perturbatively, that is, the lowest-order result estimates higher powers in the sense of an asymptotic expansion. Chosing z within an optimal window, this perturbative method yields an improved retrieval of phase information beyond mere edge detection from a single-distance intensity contrast which then is used to reconstruct the object tomographically. No assumption on the smallness of the retrieved phase needs to be made. The approach is applicable to fast phase-contrast based tomography.

Poster Number: 21

Bulk single dislocations imaging using scanning coherent x-ray diffraction

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The use of coherent x-ray beams has been greatly developing for the last twenty years, and is now used by a wide scientific community. The strength of a coherent beam is its sensitivity to phase defects. A complex speckle pattern is obtained when the illuminated volume contains many defects, out of which one can e.g. study its evolution in time (XPCS), retrieve the real space configuration performing lensless imaging, or study order/disorder transition. We will show that coherent x-ray diffraction can also be used to probe isolated phase defects in the bulk, and that the space configuration can be retrieved without any back Fourier transform calculation. This is due to the characteristic pattern obtained when such a phase defect as a dislocation line is in the middle of the illuminated volume. In that particular case, a destructive interference between out-of-phase domains takes place, resulting in a collapse of the Bragg intensity down to zero. This unique feature allowed us to image an extended dislocation line in silicon, and be sensitive to such fine structures as dislocation line dissociations in the bulk. In principle, the resolution that can be achieved by this technique is equal to the beam size. With such focusing devices as Fresnel Zone Plates or KB mirrors routinely used in synchrotrons, one could perform high-resolution mapping of dislocations in the bulk, where electron microscopy is no longer appropriate, and improve the topography technique that is limited to a resolution of about 1 micron.

Poster Number: 22

Coherent X-ray Diffractive Imaging of Strains in Crystals

Dr. Andrey Minkevich, Edwin Fohtung, Markus Riotte, Daniil Grigoriev, Taras Slobodskyy, Tilo Raumbach

ANKA, KIT

Nanoscopic elastic strain analysis is crucial for understanding physical properties and fabrication processes of crystalline nanostructures and for the application in devices. Evaluating this strain information at nanometer resolution, however, still remains a real challenge [1]. Coherent X-ray Diffraction Imaging technique based on iterative phase retrieval algorithm has the potential to solve this problem vis-a-vis directly processing the measured diffraction pattern. However, we face the problem of reconstructing a complex valued function describing the strained state of the crystal. The complex values appear under the strain induced non-centrosymmetric diffraction pattern reconstruction and their retrieval is very difficult. Under the conditions of the spatially smooth strain distribution the new modified iterative algorithm was recently developed allowing us to reconstruct the large inhomogeneous strains of order of 10-3 [2, 3]. The work presently is under progress on the incorporation of compositional variation in the samples. We will present the results of application of our method to the different diffraction patterns (simulated and experimental) from strained crystals. These results offer important perspective for local strain determination at the nanoscale. The retrieved strain field from experimental data are in excellent agreement with the analytical modelling based on elasticity theory [4].

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[2] A.A. Minkevich, M.Gailhanou, J.-S.Micha, B.Charlet, V.Chamard, O.Thomas. Phys. Rev. B 76, 104106 (2007); A.A. Minkevich, T. Baumbach, M.Gailhanou, O.Thomas. Phys. Rev. B 78, 174110 (2008).
[3] A.A. Minkevich, E. Fohtung, T. Slobodskyy, M. Riotte, D. Grigoriev, M. Schmidbauer, A.C. Irvine, V. Novak, V. Holy, T. Baumbach. Submitted (2009).
[4] E. Fohtung, A.A. Minkevich et al. Submitted (2010).

Poster Number: 23

Coherent X-Ray Diffraction Studies of Bi_2O_3 NanoIslands Using A Nanofocused X-Ray Beam

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We have used the CNM/APS Hard X-Ray Nanoprobe to measure coherent x-ray diffraction from samples of δ Bi_2O_3 nanostructures grown on single crystal surfaces of $SrTiO_3$(001). δ Bi_2O_3 is an exceptionally good oxygen conductor that could greatly improve the performance of devices relying on high ionic conductivity. Unfortunately, bulk δ Bi_2O_3 is only stable at high temperature (from ~729°C to ~825°C [1], making fabrication of such devices problematic. We have recently succeeded in stabilizing this phase at room temperature via strained, epitaxial growth [2] but the exact role of strain and defects in the growth process remain unclear. To understand these stability issues in more detail, we have measured ptychographic Bragg CXDI data from isolated islands with hard x-rays focused to a 50 nm spot and are attempting to invert this data to obtain images and strain maps. A major advantage of nanofocused x-ray coherent imaging is that subvolumes within a targeted nanostructure can be illuminated; however, understanding and modelling the interaction of a complex focused wavefront with a faceted nanocrystal requires a departure from single processor fast Fourier transform based algorithms. We are developing parallel algorithms that compute kinematic focused diffraction patterns from finely sampled model nanocrystals and are integrating these algorithms into iterative phasing routines that will converge to unique images of the structure and internal strain of individual nanocrystals. While we have not yet succeeded in inverting the data, we will present simulations that reproduce the important features of our data and suggest possible paths towards successful reconstructions.

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Poster Number: 24

Coherent X-Ray Imaging of Biomineralized Specimen

Mr. Robin N. Wilke[1], Mr. Klaus Giewekemeyer[1], Dr. Andreas Schropp[2], Prof. Christian G. Schroer[2], Mr. Adrian Mancuso[3], Mr. Jochanes Gulden[3], Dr. Ivan Vartanyants[3], Mr. Manfred Burghammer[4], Prof. Tim Saldit[1]

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We report on an high resolution CXDI experiment in the hard X-ray regime atID13 of the European Synchrotron Radiation Facility (ESRF). A focus size of 78(h)x86(v) nm2 (FWHM) has been achieved by the usage of nanofocusing refractive X-ray lenses [1]. One aim of the experiment was to study thestructure of biomineralized carbonates (CaCO3) of geobiological systems. Astrosclera w. is a model organism for biocalcification [2]. High resolution images of different contrast schemes could be readily achieved from diffraction images. CXDI techniques on weakly scattering objects such as Astrosclera w. are a challenging task. We explore possible applications.

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[2] Daniel J. Jackson, Luciana Macis, Joachim Reitner, Bernard M. Degnan, and Gert Worheide. Sponge paleogenomics reveals an ancient role for carbonic anhydrase in skeletogenesis. Science, 16(5833):1893–1895, 2007.

Poster Number: 25

Coherent X-ray Diffraction Imaging of ZnO nanostructures under Confined Illumination

Dr. Gang Xiong[1], Dr. Steven Leake[1,2], Dr. Marcus Newton[1], Dr. Xiaojing Huang[1,3], Dr. Ross Harder[3], Prof. Ian Robinson[1]

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A recently developed phase-retrieval method, known as coherent X-ray diffractive imaging (CXDI) provide a direct determination of the density of the scattering centers from the reciprocal-space distribution of the scattered intensity, and has the potential to become a powerful technique for the structural characterization of nano-sized devices[1]. The principle is based on the iterative loop of direct and inverse Fourier transformation (FT) (between the experimental intensity distribution and the sample image space) which can refine the genuine object density distribution ρ(r) even by starting from a model which is far from reality. The advantages for nanostructures investigation is that it gives 3D quantitative phase information (related to strain), as has been well presented in the works done in the last few years. However, determining the profile of the focused beam remains difficult while it is of importance of various applications of CXDI. Knowledge of the probe is a big issue for scanning methods on samples bigger than the beam. We report here the study of applying CXDI on a single ZnO nanorod and our efforts of retrieving the beam profile from a known structure. ZnO rod shaped crystals were synthesized via a chemical vapour transport and deposition technique (CVTD) on a Si substrate patterned with aluminium stripe as catalyst, which produces ZnO rod with typical length of ~1 micron and width of a couple of hundred nanometers. Measurements on thus produced ZnO nanorods were performed at the Advanced Photon Source (APS) beamline 34ID-C. The diffraction patterns were acquired by rocking curves on a direct-detection CCD and collated to form a complete 3-dimensional diffraction pattern. The resulting (010) diffraction patterns clearly show the 6-fold symmetric plane of von Laue fringes. Phase reconstruction of the diffraction data is carried out using the phase-constrained hybrid input-output (HIO) and error reduction (ER) algorithms. The focused beam was moved along the rod by adjust the height of the sample stage, so that the same measurement can be performed at different positions of the rod. The reconstructed 3D amplitude and 2D cut plane of the real-space phase image at those positions are obtained and analyzed. A phase range of ±1.57 radians was found to be sufficient to encompass the data without the occurrence of phase wrapping, this corresponds to a maximum displacement of 0.11 A. The amplitude image appears as a rounded rod crystal, with the diameter in the range of 200 nm to 220 nm along the rod, and the distance between the two ends from 600 nm to 1100 nm, depending on the measurement position. When the focused beam is located in the middle of the rod, the amplitude shows the longest distance between the ends and both ends are rough. When the beam is 0.5 micron away from the rod centre, the distance between two ends become shorter and one end of the rod is rougher while the other end is sharp. The results demonstrate the fact that when measured from the rod centre the focused beam is cutting through the rod rather than illuminating the whole crystal, while when moved away from the centre, it starts illuminating one of the ends of the rod. By reconstructing the rod shape in real space, it

is also possible to reveal the beam wavefront profile including the phase. At present our spatial resolution is around 40nm, and this will improve with better X-ray sources, focussing optics and more stable instrumentation.

[1] Ian Robinson and Ross Harder, Nat. Mater. 8, 292 (2009)

Poster Number: 26

Coherent X-ray Imaging of Paint Pigments by Scanning Phase Plate Modulator

Bo Chen[1], Fucai Zhang[2], Andrew Burgess[3], John Carrol[3], Felisa Berenguer[1], Richard Bean[1], Cameron Klewish[4], Joan Vilacomamala[4], Yong Chu[5], John Rodenburg[2], Ian Robinson[1]

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We have implemented a new coherent X-ray diffraction imaging method which scans a phase plate modulator to encode the phase through the beam transmitted by the sample. We applied this method to a decorative alkyd paint sample which contains iron oxide red pigment particles whose maximum size is 500 nm. In the experiments, a random patterned phase plate is installed in the path between the sample and the detector as a wave-front modulator. The use of a modulator reduces the dynamic range requirement of a detector and also improves the convergence of the phasing algorithm. Multiple diffraction patterns of the same illumination area on the sample are recorded as the phase plate is laterally translated to a number of positions during the measurements. The images of the paint were generated by processing the obtained diffraction patterns using a new iterative algorithm for phase retrieval. With a prior knowledge of the modulation function of the modulator, the propagation cycle of the algorithm involves 2 planes: the modulator and the detector. The experiments were carried out at Swiss Light Source. In this work, the result of a pure amplitude image is compared with an absorption contrast dominated projection from the TXM (transmission X-ray microscope) of a different region of the same sample was obtained at 32 ID-C, APS, ANL (Argonne National Laboratory). In both images, we can clearly see many black dots around 300 nm diameter which is in agreement with the size of iron oxide particles expected. This experiment is the first one using the new coherent X-ray imaging method to measure a real industrial product sample.

Poster Number: 27

Coherent X-ray Imaging of Defects in Colloidal Crystals

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Coherent X-ray Diffractive Imaging (CXDI) was applied to reveal the structure of colloidal crystals [1]. The colloidal sample was illuminated by a coherent x-ray beam through a 7 μm pinhole aperture, which was especially cleaned with a focused ion beam. The resulting diffraction patterns were measured in far field conditions with a CCD and contain several Bragg peaks and an additional interference structure between the peaks due to the coherent illumination of a finite part of the sample. The sample was investigated at two different azimuthal angles, for $\varphi = 0°$ strong Bragg peaks were observed and at $\varphi = 35°$ streaks indicating a stacking fault defect in the colloidal crystal could be seen. The inversion of these diffraction patterns, using iterative reconstruction algorithms, reveals the arrangement of colloidal particles in a face-centered cubic (fcc) lattice as well as defects in the form of stacking faults in the (111) planes. The reconstruction results are supported by additional simulations showing, that the simple and nondestructive mechanism of coherent x-ray diffraction imaging opens a unique route to determine defects in mesoscopic materials such as colloidal crystals.

[1] J. Gulden, O.M. Yefanov, A.P. Mancuso, et al., Phys. Rev. B (2010), submitted

Poster Number: 28

Coherent diffractive imaging of biological samples using phase-diversity

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We demonstrate the benefit of a phase-diversity approach to coherent diffractive imaging (CDI), based on ptychographic methods. We enhance and optimise the algorithm by using a combination of probe beam translation and variation of de-focused distance, in a Fresnel geometry. Using a lithographic test sample made of Au/Cr, we quantify the sensitivity of the method and demonstrate improved reconstructions. We present results of our phase-diverse approach applied to the adhesive produced by the tube-dwelling marine polychaete Phragmatopoma californica. The adhesive of P. californica is a proteinaceous substance, consisting of an amorphous granular nano-structure with a chemical organisation which is not completely understood. Insight into both the structure and composition of this adhesive could help with the development of a robust underwater adhesive.

Poster Number: 29

Coherent lensless imaging using UV-X harmonic beamline

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Coherent X-ray lensless imaging extends standard X-ray diffraction towards imaging of non-crystalline objects. In 2006, the first single shot ultrafast coherent diffraction pattern was measured on isolated non-periodic nano-sample [1]. More recently the same team has achieved a time resolved experiment with 100nm, 10ps space and time resolutions [2]. Up to now, this ability was limited to intense femtosecond coherent pulses from a free electron laser. High Harmonics Generation (HHG) would represent an excellent alternative since they are widely available and show the required properties to perform ultrafast coherent lensless imaging: high spatial coherence, regular wavefront, temporally coherent and of ultrashort pulse duration (femtosecond down to 100 attoseconds). Moreover, HHG pulses are synchronized on sub-femtosecond time scale with the driving infrared femtosecond laser, allowing a vast flexibility in time resolved experiments. Our approach is based on a significant improvement of UV-X yield from HHG in gases, at the microjoule level, driven in enhanced phase-matching conditions by a standard commercial femtosecond laser. A high intensity UV-X coherent beam is obtained using a loose focusing geometry, which allows coupling a very high amount of Ti:Sapphire laser system energy in the HHG process [3]. This approach allows reaching up to few 1011 photons per shot of 25 femtoseconds duration for the 25th harmonic (λ=32 nm). We first used the harmonic source for perform ultrafast coherent diffracting imaging (CDI) experiment using iterative algorithm. Reconstruction from single shot exposure of two dimensionally pure amplitude transmission object of 3 μm size has demonstrated with a spatial resolution of 120nm [4] and 80 nm more recently. We then implemented a recently proposed Fourier transform holographic technique using extended references. This technique, easy to implement, allows a direct non iterative image reconstruction. The use of an extend reference remove the limitation of the punctual reference in term of signal efficiency. Reconstruction of 2D transmission object of 2 μm size has demonstrated, in the single shot regime, with a spatial resolution of 110nm [5]. The next perspective is the using of potentiality of high temporal resolution of the HHG beamline for imaging the femtosecond dynamical organization of magnetic nano-domains [6].

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Poster Number: 30

Coherent scattering from silicon monocrystal surface

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Using coherent x-ray scattering, we evidenced atomic step roughness at the (111) vicinal surface of a silicon monocrystal of 0.05° miscut. Close to the 1/2,1/2,1/2 anti-Bragg position of the reciprocal space which is particularly sensitive to the (111) surface, the truncation rod exhibits a contrasted speckle pattern that merges into a single peak closer to the 111 Bragg peak of the bulk. The elongated shape of the speckles along the (111) direction confirms the monoatomic step sensibility of the technique. This experiment opens the way towards studies of step dynamics on crystalline surfaces.

Poster Number: 31

Crystallographic phasing of twinned microcrystals

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Twinning occurs widely in crystals and it can be a serious complication in the crystal structure determination process. When such microcrystals are illuminated coherently, the different crystallographic phases of the structure factors of the overlapping reflections will provoke interference in the form of a speckle pattern. In this communication, we will show that this 3D speckled Bragg peak distribution can be measured and provide information about the twin domains inside the crystals. Research is ongoing to invert the patterns to obtain 3D images of the twin distribution. Coherent X-ray diffraction patterns for selected manganite microcrystals were collected under a beam focussed down to 4 microns at I16 beamline of Diamond Lights Source. Three manganite compositions were chosen: Pr0.625Ca0.375MnO3, La0.625Ca0.375MnO3 and La0.275Pr0.35Ca0.375MnO3. Dispersed crystals were attached to glass and quartz capillaries by gentle heating to avoid any displacement during data collection. After centring the sample, the appropriate Bragg peaks, for instance (002), (200), (121) and (210), were identified by using the Pilatus detector and then moved onto a CCD detector with small pixel size to give sufficient resolution. The diffraction patterns were gathered by rotating the sample through the Bragg condition and subsequently collated to form complete 3D diffraction patterns. The Bragg peaks of manganites have been measured and they were broken up into fringes and speckles. This is consistent with a new theory of the connection between the twinning, a classic disorder growth mode of these materials due to the pseudocubic nature of the samples, and the phase of the domain that contributes to a given Bragg peak. It is straightforward to show that the number of speckles in the Bragg peak is equal to the number of domains in the beam. We could therefore estimate the twin domain size. Our new understanding of the origin of this speckle shows that the visibility is proportional to the phase shift between the domains. Our method represents a new way of studying twins/domains within crystals.

Poster Number: 32

Density Modification Methods for Phase Reconstruction

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Phase information is currently recovered from reciprocal-space amplitude measurements by the application of iterative projective algorithms that solve the optimisation problem. Various algorithms have been developed each of which apply constraints in real and reciprocal space on the reconstructed object. A well known example is the application of a real-space support region in which the complex density must exist. Here the object is confined spatially. Other examples include solvent flattening and flipping methods in which the complex density is confined to a subset of the complex plane. The original Sayre equation is a non-linear real-space constraint in which the real space amplitude is made equal to its squared value. All the above phase reconstruction methods rely on experimental data that is sampled above the Nyquist frequency. An important application of phasing methods is to invert Coherent X-ray Diffraction measurements to obtain images of nanocrystals. To date, support-based methods have worked well, but are less successful for highly strained structures, defined as those which contain (real-space) phase information outside the range of +/- π. This results in phase wrapping in the reconstruction which inherently contains high frequency Fourier components at the phase-wrapped intervals. Here we report on tests of a "density modification" phase reconstruction method that is not necessarily limited by the sampling frequency of the experimental data. The application of a non-linear operator in real space that confines the density bandwidth was found to significantly aid in the reconstruction of highly strained nanocrystals. In certain cases, it was also possible to reconstruct the object without the addition of the support constraint. We show how this method is able to successfully reconstruct phase information that otherwise could not be recovered.

Poster Number: 33

Detection of local symmetries in hard sphere glasses with X-ray cross-correlation analysis

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Disordered materials, such as glasses and liquids, do not exhibit translational symmetry and are thus able to accommodate different local symmetries in one and the same system. Local symmetries are not accessible in conventional X-ray diffraction experiments as the time and ensemble averaging process yields an aver-aged structure factor <S(Q)> which contains no information about local bond order . Recently it was shown that access to the local symmetries of materials is possible by applying an angular correlation function to the speckle pattern of hard sphere glasses [1]. A speckle pattern reflects the exact spatial arrangement of the particles and is accessible by a coherent X-ray beam scattered from a quasistatic disordered sample. By applying this new method to the speckle pattern of hard sphere glasses, we will demonstrate how to get a deeper insight into the local symmetries of glassy system.

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Poster Number: 34

Direct reconstruction of the illumination function for Coherent x-ray Diffraction Imaging and application to silicon-on-insulator lines

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The knowledge of strain fields inside epitaxial nanostructures is an important prerequisite to understand and tune the electronic and optical properties of semiconductor heterostructures. X-ray diffraction, using a coherent focused beam, is a powerful tool for the determination of the 3D displacement field inside nanostructures. In particular the Coherent Diffraction Imaging approach allows to recover shape and displacement fields directly from the coherent and oversampled Bragg scattering intensity by applying inversion iterative algorithms [1,2]. The precise knowledge of the illumination function is an essential part of this approach, as the retrieved phase of the wavefield at the sample position includes contributions from both the illumination wavefield, as well as the displacements within the studied nanostructure. These two contributions have to be disentangled for the correct interpretation of displacements [3,4]. We will show the last results that we obtained from the characterization of the wavefront, in particular the ab initio reconstruction of amplitude and phase of the x-ray beam at the focal position of a Fresnel Zone Plate using the far-field intensity pattern in the divergent part of the focused coherent beam [5]. Finally we will discuss how this influences the imaging of the displacement field in strained nanostructures, in the particular case of strained silicon-on-insulator (sSOI) lines.

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Poster Number: 35

Dose requirements for resolving a given feature in an object by coherent x-ray diffraction imaging

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We address the question of what dose is required to image an object by coherent x-ray diffraction imaging (CXDI) and to resolve a certain sub-unit or feature of that object. We show that a necessary condition for being able to resolve the detail is that the feature could be imaged by itself. The quality of the reconstruction of the feature is nearly independent of the surrounding, whether it is embedded in a larger object or not. This allows one to easily estimate the dose requirements for identifying atoms and clusters in larger objects. We illustrate the result by a numerical example and give an estimate for the dose required to resolve single atoms of different elemental species in CXDI experiments at free-electron laser and synchrotron radiation sources.

Poster Number: 36

Effects of environment cell x-ray windows on Coherent X-ray Diffraction Imaging

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One of the significant advantages of lensless Coherent X-ray Diffraction imaging is that optics are not required near the sample. This freedom has opened the possibility of high resolution imaging of samples in varied environmental chambers. Particularly in the Bragg geometry, where the coherent scattering in the vicinity of Bragg peaks is measured, these coherent diffraction measurements are relatively insensitive to parasitic scattering that arises from the x-ray windows of an experimental chamber. For this reason, a variety of studies have been started relying on in-situ and in-operando experiments on crystalline samples contained in cryostats with beryllium domes, catalysis chambers with Kapton film windows and diamond anvil cells with thick beryllium gaskets. While these measurements are not subjected to strong parasitic scattering, defects within these windows often give rise to aberrations in the scattered wave front that distort our measured diffraction patterns. To test the effect these aberrations have on the reconstructions of coherent diffraction patterns to images, we performed coherent x-ray diffraction measurements around the 111 Bragg peak of a nanocrystal of gold. The identical particle was measured both from within and without a typical helium flow cryostat beryllium dome. The results of these experiments will be discussed, as well as simulations done to investigate the limits of our sensitivity to such artifacts.

Summary:
When coherent x-ray diffraction imaging is done of samples within environmental cells, the x-ray windows introduce aberrations into the diffracted wave front. We have studied the impact of these aberrations on reconstructions of the measured diffraction pattern to images. An experiment done with a gold nano crystal and beryllium dome will be discussed and simulations to investigate the limits of such measurements will be shown.

Poster Number: 37

Finite-Element-Method Simulations of Strains for Gold and ZnO nano-crystals

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Finite-Element-Method Simulations of Strains for Gold and ZnO nano-crystals Xiaowen Shi, Gang Xiong and Ian Robinson London Centre for Nanotechnology, University College London, U.K. Finite-element-analysis (FEA) is a very good tool for theoretical studies on strained nanostructure materials, useful to understand the strains seen in coherent X-ray diffraction experiments. FEA is also a useful way to simulate strain patterns of nanostructure electronic devices under both fabricating and operating conditions. Here we report our studies on strained induced by chemical coating of gold nanocrystal and highly-strained ZnO nanocrystal by using the COMSOL multi-physicsR simulation package. The results are compared with measurements which were conducted at beam line ID-34 at Advanced Photon Source, Argonne National Laboratory, IL, US[ref: our joint paper]. Strain displacements were simulated by COMSOL Multi-physicsR with continuum elasticity calculations. We simulated strain patterns on facetted gold sphere of 300nm in diameter in contact with a thin skin of the same material (gold) of thickness of 5nm with isotropic stress of 0.38GPa on both the top and the bottom facets. Differential surface stress was generated by applying zero stress on curved spherical surface regions on the object. The macroscopic elasticity coefficient of Gold is used. The displacement fields (strain components) in all 3 directions on the object, were recorded to generate 3D calculated diffraction patterns by performing Fast Fourier Transforms on the complex density functions of the simulated object with the phase factor being the dot product of the displacement fields and the selected reciprocal lattice vector to be determined by incident and outgoing X-ray wave vectors. The real space phase shift is the projection of the displacement of atomic positions of the crystal from an ideal lattice onto the reciprocal lattice vector selected. Furthermore, we report simulations of diffraction patterns on highly-strained ZnO nanocrystal by using COMSOL Multiphysics^{R}. Highly-strained diffraction patterns were generated by introduction of large phase shifts which were generated by setting the thermal expansion coefficient of the polycrystalline substrate to be zero so that the mismatches of thermal expansion coefficients of the gold nanocrystal and ist substrate induces strain patterns when higher temperature is applied to the system.

Poster Number: 38

Fresnel coherent diffractive imaging: Pollen grain reconstruction

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Fresnel coherent diffractive imaging (FCDI) is a relatively recent technique for structure determination. This technique has some advantages over other coherent diffractive techniques. The "holographic" region that results from interference of the incident beam with the sample's exit-surface wave (ESW) makes possible to recover an image from it by back propagating from the detector to the sample. This technique was applied to investigate a region of a single pollen grain. The experiment was performed at the Advanced Photon Source on beamline 2-ID-B which provided 1820 eV photons (6.8 A) using a spherical grating monochromator. A Fresnel zone plate (diameter 160 μm and outermost zone width 40 nm) was used to create the diverging beam required. FCDI data from the extremity of a pollen grain with a size of 4 μm was measured. To reconstruct an image, two types of measurement are required. The 'white-field' data are collected without a sample in the path of the beam and used to recover the complex illuminating wave. The ESW data are collected when the sample is placed in the x-ray beam and are used in the iterative scheme, in conjunction with the recovered complex illumination, to phase the ESW in the detector. This phased ESW may then be inverted to yield an image of this region of the pollen grain. We show a reconstruction of a region of a single pollen grain with FCDI. We note that the features observed concord with those expected, given current knowledge of plant biology, and that this technique, in particular extended to three dimensional imaging through tomography, shows promise for future high resolution bio-imaging of cell-sized samples with coherent x-rays.

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Poster Number: 39

Hard X-Ray Phase Contrast Imaging of Black Lipid Membranes

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Membranes are considered as the most important interfaces in biology, and can be visualized under physiological conditions by optical techniques such as phase contrast and fluorescence light microscopy. While the contour lines and large lateral domains of biological membranes can be imaged, the density profile of the membrane and associated changes cannot be resolved by visible light. We report on hard x-ray phase contrast imaging of black lipid membranes (BLMs) [1], which are freely suspended over a micro machined aperture in an aqueous solution [2]. This new way of membrane structure analysis allows investigating bio molecular and organic substances in aqueous environments by parallel and divergent beam propagation imaging, using partially coherent multi-keV x-ray radiation [3-5]. The width of the thinning film is significantly smaller than the detector pixel size, but can be resolved from quantitative analysis of the intensity fringes in the Fresnel diffraction regime down to its native thickness of about 5nm [6]. We have put forward a simplified but extendable model, which enables the theoretical description of image formation and thus the characterization of membrane thickness and its decrease during the thinning process from a bulk to a bimolecular film. The structural changes can be obtained from both the loss of contrast and the asymmetry of the detected Fresnel fringes. On the basis of the recent experiments, future investigations will be performed to study the interactions of membranes, as they are for example known from synaptic fusion, with high spatial resolution.

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Poster Number: 40

High-fidelity Reconstructions in X-ray Diffraction Microscopy

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The post-experiment processing of data in x-ray diffraction microscopy is often time-consuming and difficult. This is mostly due to the fact that even if a preliminary result has been reconstructed, there is no definitive answer as to whether or not a better result with more consistently retrieved phases can still be obtained. We show that the first step in data analysis (the assembly of two-dimensional diffraction patterns from a large set of raw diffraction data) is crucial to obtaining reconstructions of highest possible quality, such as have been published recently [1]. We have developed software that automates this process and results in consistently accurate diffraction patterns. A common tool to assess the quality of a reconstruction is the phase retrieval transfer function (PRTF). However, this measure is used with great variability in the literature, with different groups using different values of the PRTF to judge their resolution cutoff. We show that incorporation of a Wiener filter improves the PRTF's interpretability and utility for judging reconstruction quality and we look into how averaging affects the validity of the PRTF curve. Both developments are important steps towards a more guided phase retrieval process.

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Poster Number: 41

Imaging magnetic domains by resonant Fresnel coherent diffraction

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We studied the domain structure in a ferrimagnetic GdFe multilayer by resonant Fresnel coherent diffractive imaging (FCDI). Contrast sensitive to the magnetic moment of the domains was achieved by taking advantage of x-ray magnetic circular dichroism at the M-edges of Gd. Because linearly polarized illumination was used, no interference between the magnetically scattered and unscattered waves was observed. Compared to plane-wave coherent diffraction, significant real-space information about the sample can be seen in the Fresnel region of diffraction data obtained by FCDI. In our experiments, highly magnified images of the domains were visible within this region, with significant diffraction outside it. The magnetic scattering contrast was so high that we could trace the evolution of the domain walls as a magnetic field was applied. In this paper, we present reconstructions of resonant FCDI data showing the domain structure in the GdFe multilayer system at better than 30 nm resolution. We discuss the meaning of phase shifts in the reconstructed images.

Poster Number: 42

Magnetic domain dynamics in Fe/Gd magnetic multilayers

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We study the evolution of magnetic domains and effect of pinning centers in thin film magnetic systems as a function of magnetic field and dopants to identify the role the disorder in formation and stability of the domains in these systems. We have studied Fe/Gd multilayer exhibiting ordered stripes due to perpendicular magnetic anisotropy (PMA). We study the effects of field pinning of the local magnetic structure of these systems through their magnetization hysteresis loops both along easy and hard axis of magnetization. Using element sensitivity and depth resolution of resonant magnetic x-ray coherent scattering technique we investigate the magnetic domain structure and intermittent switching dynamics. Comparison of the magnetic speckles (in momentum space) provides information on correlation between the magnetic structures (in real space). We will present the X-ray Coherent Speckle Metrology approach to study Barkhausen noise spectrum as a function of the applied magnetic field, and will discuss extension of this study to Tb-doped Fe/Gd magnetic films.

Poster Number: 43

Magnetic imaging at linearly polarized x-ray sources

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Resonant magnetic scattering can change the polarization state of x-rays. In experiments utilizing interference between a magnetic sample and a reference beam such as holographic imaging or heterodyne detection of XPCS, control of the polarization of the incident coherent x-ray beam is mandatory to ensure the possibility of interference at the detector. So far, the existing x-ray FELs exclusively generate linearly polarized radiation. We present polarizers for these sources based on dichroic x-ray absorption allowing the generation of elliptically polarized x-rays. The devices will enable the use of ultra-short circularly polarized x-ray pulses for polarization dependent single and multi-shot experiments at present FEL sources. We compare and characterize multilayer and single thin film polarizers and present images of magnetic nanostructures recorded by Fourier Transform holography using this approach. Based on the results, a polarizer-setup to be integrated into the SXR beamline at LCLS will be presented.

Poster Number: 44

Interpreting anisotropic diffraction patterns from aligned ensembles

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On ultrashort time scales, excitation of molecules by a linearly polarized laser field always produces aligned ensembles. If we want to subsequently probe the dynamics or image the molecules with ultrafast diffraction, we need to account for this anisotropy. From previous studies, it is known how to systematically break down the two-dimensional diffraction pattern into a set of one-dimensional scattering curves. We have studied the information content in these curves, and calculated the diffraction patterns for NaI excited by a uv laser.

Poster Number: 45

Lensless imaging with direct inversion: Generalizations to Fourier Transform Holography and optical proof-of-concept experiments

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Lensless imaging has become a key technique in coherent x-ray microscopy when optics, such as lenses, zone plates or mirrors are not available or difficult to manufacture. Unless scanning techniques are applied, the lensless approach leads to analyzing diffraction images and imposes the common phase problem of coherent diffraction imaging. Throughout the last two decades, numerical iterative algorithms have found great interest and have advanced far in addressing the phase problem. However, some questions have remained regarding the uniqueness of a solution or the convergence of the algorithms. Holographic methods may become a promising alternative, as they can provide direct one-step solutions to experimental diffraction data. A recent holographic technique for CDI combines differential operation with Fourier Transform Holography by using a polynomial to weigh the diffraction data prior to the Fourier transform. Polynomial Weight Fourier Transform Holography (PWFTH or HERALDO) has been theoretically proven for certain holographic references in 2007. Experiments were published shortly after using optical laser sources where we demonstrated the experimental and theoretical applicance of PWFTH to phase shifting references. We will present this result which, we think, is important for future x-ray experiments. So far, only a small variation of reference structures have been used for PWFTH and a greater variety of possible references may be needed for future experiments. Therefore, we also present a current result which is a general analytical solution. It generates an entire class of possible holographic reference structures and includes the references used so far in theory or experiment as low-order cases.
We present theoretical and experimental findings findings for a recent holographic technique which is based on Fourier Transform Holography.

Poster Number: 46

Measurement of Wavefront Curvature and Spatial Coherence of Electron Beams by Using a Small Aperture

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In diffractive imaging, electron and x-ray beams are generally assumed to be coherent plane waves. In reality, electron beams in transmission electron microscopes (TEM) are partially spatially coherent and their wavefronts are curved. Although we must optimize illumination lens conditions for electron diffractive imaging [1], there are few reports on measurement of wavefront curvature and spatial coherence of beams in TEM. In the present study, we propose a new technique for measuring them by using a small aperture [2] which selects an area about 3 nm in diameter in a sample plane. First, we have measured wavefront curvature of beams by using the small aperture. When the aperture is inserted in a beam, a position of the direct spot in a diffraction pattern reflects an average of travelling directions of the beam passing through the aperture. We measured shifts of the direct spot when the aperture was moved in a beam. By using the results, we succeeded in calculating phase distributions of the beams with different diameters. Next, we have measured spatial coherence of the beams. When we use a small aperture, we can measure the direct spot convolved with the Airy pattern. When the incident beam is partially spatially coherent, the pattern is blurred as the result of the convolution with an extended source. By deconvolving the blurred Airy pattern, we obtained degree of coherence as a function of distance between two points in a beam on the basis of the van Cittert-Zernike theorem. The result shows that coherence lengths are only a small percent of beam diameters. We succeeded in measuring both wavefront curvature and spatial coherence. These results will be useful for various precise measurements in TEM including diffractive imaging.

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Poster Number: 47

Motion correction in Fresnel Coherent Diffractive Imaging

Mr. Jesse Clark[1], Dr. Garth Williams[2], Mr. Corey Putkunz[1], Prof. Keith Nugent[3], Dr. Harry Quiney[3], Dr. David Vine[3], Dr. Ian MCNulty[4], Dr. Andrew Peele[1]

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Fresnel Coherent Diffractive Imaging uses illumination with wavefront curvature to improve the robustness and reliability of the reconstruction process in Coherent Diffractive Imaging. Motion of a sample with respect to the illumination can make it difficult to combine diffraction images to increase signal to noise. We present a method to account for relative sample-optics motion ex post facto through modifications to the phase retrieval algorithm. The new algorithm allows a reconstruction to be obtained from multiple or single diffraction patterns that have been degraded by relative motion. Incomplete or partial knowledge of the motion can be overcome by modelling the motion. The algorithm can also be generalised to account for other experimental nuisances such as time varying illumination.

Poster Number: 48

Nanofocused synchrotron radiation Bragg diffraction on Nanowires

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The unique electronic, optical, and structural properties of semiconductor nanowires (NWs) allow the fabrication of suitable building blocks for future nanoelectronic and nanophotonic devices [1–3]. Such applications require complex NW structures with either axial or radial heterostructures. Powerful structural analysis tools to access the dimensions and strain states are crucial to optimize heterostructured NW growth. X-ray diffraction has been successfully used to deduce the average structural and chemical parameters [4]. We recently reported the determination of these parameters in ensembles of InAs/InAsP core-shell NWs grown on Silicon substrates [5]. This methods require NW ensembles with a narrow distribution of shape and composition, which is also desired for many NW applications. Basic research, however, additionally requires insight into single NWs, or even parts of them as the NW-substrate interface, to complement information from other methods like transmission electron microscopy, where sample preparation is difficult and often destructive. We have used focused coherent synchrotron radiation Bragg diffraction to investigate single NWs, both ”simple” InAs NWs as well as InAs/InAsP core-shell wires with a phosphor concentration of 26 % [5]. Using standard phase retrieval algorithms[6, 7], we derived the scattering density of the InAs NW [8]. Deriving the complex scattering density of a strained core-shell NWs without using a priori information of the investigated object (like in the case of Minkevich et al.[9]) was not successful so far. In order to develop better algorithms and/or measurement methods, to improve convergence, we have therefore worked on simulated data from model structures with the same geometry, but with smaller strain values as present in the measured NWs. The convergence for strained NWs is very poor when using only the so-called support constraint in real space, since the amount of unknown information increases tremendously when the phase of the measured electromagnetic field is varying in a wide range of angular space. Using a variation of the guided hybrid input-output[10] algorithm along with the shrink-wrap algorithm[7], and a proper value for the feedback parameter β outside the usual range (see [11]), the convergence for weakly strained test objects was investigated: By applying internal constraints like the positivity of the real part of the real space scattering density (corresponding to limiting the phase in real space to the range of -π/2 to π/2), weakly strained core-shell NW were retrieved up to an error (see Ref. [10]) of 10^(−15) . When probing the (111) Bragg reflection, the treshold of the P concentration for having a phase shift within the mentioned range is at about 2.5 %. For phase retrieval without using such internal constraints, convergence is already an issue for non-strained objects, and becomes poorer and poorer for increasing strain values, and hence range of phase variation. The question where the limits of current algorithms lie, and whether it is in practise possible to retrieve highly strained objects without a priori

information, remains open. Beside possible improvements of phase retrieval algorithms, also the measurement schemes may be adapted. Measuring several near field intensities, or measuring several Bragg reflections, where the strain in one of the scattering directions is very small, are some suggestions. We will discuss the effect of such schemes on retrieval of our strained test objects.

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Poster Number: 49

Orientation Determination in Single Particle X-Ray Coherent Imaging

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X-ray single particle imaging [1] is a very promising technique for the determination of reproducible biological specimens' structure. It is expected to allow high resolution structure determination for samples that cannot be crystalized. The main idea suggests injecting similar particles in unknown orientations into the FEL beam [2]. Through an analysis of the diffraction patterns, the corresponding specimen orientation for each measurement can be determined and a full 3D reciprocal space can be obtained. By applying a phase retrieval technique to this reciprocal space, the electron density distribution inside the sample can be reconstructed. We proposed to use an algorithm for the orientation of single particles determination, which is based on the fact that all diffraction patterns represent spherical sections of the reciprocal space through its origin. Thus all patterns intersect all other patterns along some arcs. As the intensity along an intersection curve is identical for both intersecting patterns, the unique positional relationship of two patterns under consideration can be determined. Simultaneous analysis of the common arcs for several patterns gives the possibility to use the common arc approach for noisy data with a small number of diffracted photons, which is the case even for ultra bright XFELs [3]. We have also proposed a way of selecting the right order of patterns processing and a way of checking the orientations during 3D reciprocal space assembly. The algorithm was tested on two different biological structures, 20-30 nm in size, one of which was a virus with icosahedra symmetry, and the other an artificially made asymmetrical structure. The wavelength of the incident x-ray radiation was chosen to be 3A and the flux 1012 photons focused into 100x100 nm2 spot with Poisson statistics applied to the detected signal. The calculated patterns had a very low flux, of about 0.05-0.15 photons per pixel at the outer edge of the detector, and the resolution of the initial patterns was about 4 nm. The resulting 3D reciprocal space, constructed from more then 10 000 patterns, had a resolution of about 3.3A. The algorithm of orientation determination proposed has several very important advantages when compared with the other approaches [4, 5, 6]. It is linearly scalable with the number of measured patterns and the number of pixels in the diffraction patterns. It doesn't require classification of the patterns [6], which can lead to additional error. Importantly the algorithm is easy to parallelize, because most of the calculations are independent. It has minimal RAM requirements, because the data can be processed in parts.

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Poster Number: 50

Probing of strain in nanostructures by indirect and direct methods

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X-ray coherent diffraction imaging [1, 2] is a well known model free approach for imaging of small nano-particles (including internal). At this scale, the detailed knowledge of the structure plays a major role in the determination and understanding of related physical properties. The question of the internal strain field distribution remains especially challenging. It requires not only a high sensitivity to atomic positions with a nanometre resolution but also the capability to analyze as many as 104-1010 atoms to investigate crystal with size in the 10-1000 nm range. Although the electron based diffraction techniques present an excellent resolution, a great advantage of diffraction with x-rays results from their weak interaction with matter, leading to non-destructive investigations of bulk materials. However, due to the lack of x-ray lenses for direct imaging, the analysis of the intensity pattern is strongly model dependant. In this context, lens-less x-ray imaging techniques are highly desirable as they combine the sensitivity of x-rays with a model free analysis. On the other-hand, analytical model based methods will be highly advantageous as when combined with the phase retrieval technique to provide a complete picture of the strain tensors. We report on results obtained from our newly developed analytical method [3] to image elastic deformations in III-IV device based materials. The obtained strain field are in excellent agreement with those obtained from FEM and CXDI [4]. In general, highly complementary information from the different approaches is much more powerful when used together.

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Poster Number: 51

Reconstruction of surface morphology from coherent reflectivity of white x-ray beam

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Static speckle measurements are performed using white x-rays at the bending magnet EDR (Energy Dispersive Reflectometry) beamline at BESSYII [1]. A triangular shaped Si wafer is illuminated by coherent white x-rays by making the illuminated sample length stepwise larger or smaller compared to the beam footprint where the oversampling condition can be satisfied (Fig. 1). All other parameters of the experiment kept unchanged. At position 1 the sample width along the beam direction was larger than the beam-footprint. At position 2 the sample width (~2.3 mm) was slightly smaller than the footprint (~2.86 mm). At position 3 the sample width of ~ 0.8 mm was less than the half of the footprint. This satisfies the support constraint with the oversampling ratio $\sigma = 3.5$. For the reconstruction of surface profile the commonly used phase retrieval algorithms are modified by including illumination function [1] and propagator term. The reconstruction at different x-ray energies gives reproducible profile information at different depth of the sample depending on the penetration depth of x-rays at the energy (Fig. 2) [2]. The relative variation of local height in the reconstructed surface profiles show gradual decrease from lower (8 keV) to higher energies (12 keV). Also the roughness of the reconstructed height profiles at lower energies is higher compared to higher energies. This can be attributed to the fact than the roughness features caused by preparation of triangular sample are more pronounced near the surface of the sample and have less influence for the region inside the bulk of the sample.

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Poster Number: 52

Single Shot Soft X-ray Holography using Extended Reference

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X-ray lensless imaging is demonstrating a very high potential in performing images of isolated nanoscale objects with unprecedented space and time resolution. Active research is currently pursued to push the capability of this technique using coherent X-ray sources recently available. In this context, we present a Fourier transform holographic configuration using an extended reference [1]. Major advances shown here rely on high signal efficiency and on the direct image reconstruction process of the object performed by a simple linear derivative and a Fourier transform. We extend the demonstration previously done in the infrared [2] to soft X-ray wavelengths. Single shot imaging has been achieved with a table top soft X-ray source based on the high order laser harmonics generation process [3]. A spatial resolution of 110 nm is obtained with an integration time of 20 fs.

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Poster Number: 53

Soft x-ray holographic microscopy

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We present a new x-ray microscopy technique based on Fourier transform holography (FTH). In the original FTH experiment for magnetic imaging the field-of-view is fixed to the sample [1]. The main feature of our concept is that the sample is separated from the field-of-view-defining holography mask [2]. This allows the sample to be shifted relative to the mask, thus large samples can be imaged by combining several field-of-views. Since this extends FTH into a true microscopy technique, we name it x-ray holographic microscopy (XHM). The setup consists of two SiN membranes in close contact that can be positioned with nm-precision with respect to each other. The membrane facing the incoming x-ray beam carries the mask while the sample is prepared on the downstream membrane. For magnetic samples based on 3d transition elements, element selectivity and magnetic contrast is obtained from the x-ray magnetic circular dichroism at the L3 absorption edge. We demonstrate the power of XHM by studying the laterally varying magnetic domain structure in a Co/Pt as function of locally varied Fe overlayer thickness.

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Poster Number: 54

Strain and stacking faults in sub-100nm nanowires using coherent Bragg imaging

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Coherent Diffraction Imaging is a promising technique for the three-dimensional study of single objects using coherent X-ray nano-beams. This technique, when used on Bragg reflections [1-5], can be used to recover both the shape and strain inside the objects. In semi-conductor nanowires (NWs), the knowledge of the exact strain state is essential for the tuning of the physical properties (conduction, photo-emission). While ensemble-averaged studies can provide quantitative information about the shape and strain state [6], this is only possible in the case of a very low dispersion of the structural properties. This presentation will be focused on the study of small (diameter<100nm) homogeneous and heterogeneous NWs, which have been studied using Coherent Bragg Imaging (CBI) [7,8]. One of the issues often encountered for NWs is the presence of stacking faults, particularly for wurtzite or zincblende structural types: such faults are equivalent to a shift (or mirror image) of the lattice, and can transform an homogeneous NW into a phase object, whose domain structure can then be reconstructed ab initio. In the case where only a few stacking faults are present, they can also create artificial holes in the reconstructed electronic density [8], due to the limited real-space resolution of the reconstruction. In the case of heterogeneous nanowires, we will show that it is possible to use the small size of existing nano-beams (e.g. 300x500 nm^2 using a Fresnel Zone Plate on beamline ID01@ESRF) to perform CBI measurements on different parts of an heterogeneous InSb/InP NW, and therefore analyze the strain state near the interface. Finally we will discuss the current challenges presented by the method: (i) the requirement to determine the amplitude and phase of the incident focused X-ray beam, (ii) the difficulties of keeping a single object inside a nano-beam while rotating it over ~1° to record the 3D scattering pattern , and (iii) the effects of radiation damage due to the high flux (>10^4 ph/s/nm^2) on the sample.

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Poster Number: 55

Strain in epitaxial nanostructures: a feasibility study

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Nanoscaled epitaxial semiconductor heterostructures are systems where strain can be used to tailor the electrical and optical properties of materials. The determination of 3D atomic displacements at the nanoscale is thus an important task and still remains a challenge. X-ray diffraction is successfully applied to characterize the displacement fields in nanostructures assemblies, as long as the ensemble average information is representative of the single nanostructures. The limit is reached with self-organized grown semiconductor nanostructures, with large distribution of structural properties. Therefore, single objects characterisation approaches are required, with highly sophisticated setups, using nanofocused x-ray beams and mechanical positioning with nm precision [1]. We are developing iterative phase retrieval algorithms to study highly strained epitaxial nanostructures by Coherent Diffraction Imaging. Despite the great progress of phase retrieval approaches for the strain determination of isolated nanostructures [2], obtaining a full 3D structural information of epitaxial nano-objects is still a challenge and is dependent on the specific case [3]. In this talk, we present a feasibility study applied to a model system: SiGe nano-pyramids epitaxially grown on Si substrates. We address the specific issues arising from the application of phase retrieval algorithms to epitaxial systems, where the scattered field contributions of both the nanostructure and the strained substrate are interfering. We discuss the applicability of phase retrieval algorithms to these systems, using numerical simulations from FEM calculations, and show an example of a successful reconstruction [4].
We discuss the applicability of phase retrieval algorithms to epitaxial nanostructures, where large strain fields and susbtrate contribution make the CDI approach a very challenging task. We use numerical simulations from FEM calculations, and show an example of a successful reconstruction.

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Poster Number: 56

Thomson scattering on inhomogeneous targets

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The introduction of brilliant free electron lasers enables new pump-probe experiments to characterize warm dense matter states. For instance, a short-pulse optical laser irradiates a liquid hydrogen jet that is subsequently probed with brilliant soft X-ray radiation. The strongly inhomogeneous plasma prepared by the optical laser is characterized with particle-in-cell simulations. The interaction of the soft X-ray probe radiation with the inhomogeneous plasma is also taken into account via radiative hydrodynamic simulations. We calculate the respective scattering spectrum based on the Born-Mermin approximation for the dynamic structure factor considering the full density and temperature dependent Thomson scattering cross section throughout the target. We can identify Plasmon modes that are generated in different target regions. Therefore, such pump-probe experiments are promising tools to measure not only the important plasma parameters density and temperature but also to gain valuable information about their profile through the target. The method described here can be applied to various pump-probe scenarios by combining optical lasers, soft X-ray as well as X-ray sources.

Poster Number: 57

Wave optics simulations towards the exact modelling of Zernike phase contrast X-ray microscope based on discrete phase shifter.

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In order to gain understanding essential for the correct interpretation of Zernike phase contrast images produced by the full-field X-ray microscope [1] at the TOMCAT beamline of the Swiss Light Source we are developing an exact model to simulate this complex instrument. The complexity dwells in the choice of using an in-house developed square beamshaping condenser lens [2] and in turn a discrete array of Zernike phase shifting elements. The imaging properties of the microscope benefit substantially from the unique characteristics of both of these optical components. Meanwhile, their relatively complex structure imposes obstacles in our effort to retrieve the phase information in a quantitative manner. The knowledge of the wavefront propagating from the condenser to the detector can provide a tool which is useful in describing the image formation when operating the X-ray microscope in absorption, but most importantly in Zernike phase-contrast mode. Our approach is based on the description of the diffraction at each optical element, calculating the illumination at the sample in the focal plane of the condenser and the wavefront downstream the objective zone-plate followed by an array of micro-pillars acting as a Zernike phasing element. The methods and current results of the simulations will be discussed as well as examples of radiographic and tomographic phase contrast images will be presented.

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Poster Number: 58

Sub-15 nm beam confinement by two crossed x-ray waveguides

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X-ray waveguides can be used to filter short wavelength radiation at nanoscale dimensions, replacing the function of macroscopic slits and pinholes used in conventional x-ray experiments. Waveguides can thus provide localized and highly coherent beams for diffraction studies at significantly reduced sample volume, as well as for coherent x-ray imaging and holography. We have combined two high transmission planar x-ray waveguides glued onto each other in a crossed geometry to form an effective quasi-point source [1, 2]. From measurements of the far-field diffraction pattern, the phase and amplitude of the near-field distribution is retrieved using the error-reduction algorithm. In agreement with finite difference field simulations (forward calculation), the reconstructed exit wave intensity distribution (inverse calculation) exhibits a full width at half maxi-mum (FWHM) below 15 nm in both dimensions. Holographic imaging is successfully demonstrated for the crossed waveguide device by translation of a lithographic test structure through the waveguide beam [2]. Further, we have realized waveguide-based x-ray microscopy of unstained biological cells [3].

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Poster Number: 59

Theoretical Analysis of Disordered Systems Structure by Angular Cross-correlations in Coherent X-ray Scattering Experiments

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The microscopic understanding of the structure of matter is of fundamental importance for materials design. Complexity in the structure is often associated with a sophisticated functionality of materials. Thus, study of the structural properties of complex matter is a challenging task for materials science on the way to development of high performance materials. Significant progress in theoretical studies of magnetic, electronic and other properties of the crystalline matter has been achieved due to the applicability of powerful and relatively simple description of the crystals structure. Opposite to crystals, the concepts used for description of microscopic structural properties of such complex materials as liquids and glasses did not go far beyond the pair distribution function [1-3]. This is an unfortunate gap considering that disordered matter may exhibit novel complex functional properties. Availability of the state-of-the-art X-ray sources with the high degree of transverse coherence together with the recently developed experimental methods enable new possibilities to access the microscopic structure of disordered matter. Application of the angular cross-correlation functions (CCF's) to the results of coherent x-ray scattering experiment made possible to reveal local symmetries in disordered systems [4]. We propose a general theoretical basis for the angular CCF, covering a wide range of structural properties in disordered systems, from local symmetries to spatial correlations between distant structural elements. Here we present the results of simulations of coherent x-ray scattering on disordered systems. We consider molecular gas as a model system representing disordered matter. We elucidate the relation between spatial correlations in disordered systems and properties of the intensity CCF's.

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Poster Number: 60

Visualising local defects in Au nanocrystals with Coherent X-ray Diffraction Imaging

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We are interested in the strains that appear in small crystals, considering that these strains are the origin of new and interesting properties of nanomaterials. Gold is a highly useful, strongly x-ray scattering material with many applications, ideal for investigation in CXDI experiments. Using the Coherent X-ray Diffraction beamline at 34-ID C, APS, a 250nm sized crystal was aligned inside a focussed X-ray beam in three dimensions with the aid of an in situ confocal microscope. A total of 6 Bragg reflections in reciprocal space were successfully measured from a single crystal. Three further reflections were obtained from a twin domain within the same crystal. The diffraction patterns were inverted and phase information (lost during measurement) recovered by oversampling data and utilising a support based Hybrid-Input-Output algorithm. The recovered phase is a projection of the displacement field onto the direction of the Q-vector which allows visualisation of defects within the crystal. Simulations have been carried out using finite element analysis software, COMSOL which display the observed defects. Both simulations and reconstructions confirm there to be a significant strain associated with twin boundaries. Reconstructed phase information and the recovered complex amplitude from multiple reflections have enabled the clear identification of slip bands within the crystal likely formed during sample preparation, when a small amount of Au film is annealed on a SiO_2 substrate in order to create individual nanocrystals. The film volume has been found to play an important role in the observed strain in fully annealed crystals. Strategic sample preparations used in conjunction with a confocal microscope in-situ enabled three-dimensional sample alignment to overcome sphere-of-confusion issues when locating Bragg peaks in reciprocal space. The confocal alignment method enables a full determination of the strain tensor with three or more Bragg reflections from the same crystal. It will also crystalline defects to be studied by measuring unstrained crystals before and after damage is purposefully induced in them e.g by Focussed Ion Beam or Laser Shock heating.
https://docs.google.com/fileview?id=0B_obk6-36aAeMzQ4ZGE3NGUtYmU2ZC00ZDk4LTliOTItZDljYTNjNjFmY2Y1

Poster Number: 61

X-ray cross correlation analysis and the effects of limited Q information

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Current simulations of disordered matter and experiments using the newly developed X-ray cross correlation analysis, XCCA, have taken place using all information available along a constant and angularly continuous momentum transfer, Q; taking the direct beam as a reference point and considering a two-dimensional detector. Such an approach has used the average of the intensity-intensity correlations along this path with constant modulus Q and fixed angular offset, and enabled extraction of local symmetries that would not be accessible through a more traditional pair-correlation function paradigm. For large momentum transfers, as is the case for molecular liquids and glasses, there are at present no 2-D detectors available to cover the equivalent angular Q-range. Therefore, it is necessary to study the effects of angularly discontinuous data along a constant Q on the ability to still be able to extract local orientational correlations.

Poster Number: 62

Coherence Measurement using Iterative Techniques

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It is in the interests of all those working in the field of X-ray imaging using synchrotron and XFEL sources to achieve the highest possible efficiency and resolution in their work. Strictly demanding fully coherent illumination of the sample to be imaged can result in a reduced photon flux incident upon the sample, as is the case especially for larger samples. Recently published work[1] has demonstrated that the error reduction algorithm for iterative phase retrieval can be generalised for use with partially coherent illumination, provided the coherence properties of the beam are known a-priori. Most readers will be familiar with the method of measuring the beam coherence by means of a Young's interference experiment. Such measurements are capable of only probing the coherence properties of a beam at discrete points in the beam. A more general measurement of the coherence properties may be obtained by recording the diffraction patterns at a number of distances downstream from an aperture, and mathematically combining the diffraction patterns to obtain a characterisation of the coherence properties of the entire beam across the aperture. We used the coherent mode expansion [2] as a means of expressing the coherence properties of the incident beam as linear combination of coherent modes, and expressed each coherent mode as a linear combination of orthogonal Legendre polynomials. The coefficients of each Legendre polynomial in the expansion were adjusted by means of a Newton-Raphson procedure to optimise the fit to the experimental data, thus achieving a characterisation of the coherence properties of the beam. This method was applied to both simulated and experimental synchrotron data taken from an intermediate energy X-ray undulator beam at the Advanced Photon Source. The simulations were performed to quantify the data quality requirements for retrieving coherence information in excess of that which could be gained from performing interferometric experiments. The simulations suggested that the noise present in our experimental data would suppress any coherence information which could not have been gained from an interferometric measurement, and our analysis of the experimental data demonstrated that this occurred.

Poster Number: 63

Coherence Properties of Hard X-ray Synchrotron Sources and X-ray Free Electron Lasers.

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HASYLAB at DESY

A general theoretical approach based on the results of statistical optics is used for the analysis of the transverse coherence properties of 3-rd generation hard x-ray synchrotron sources and x-ray free-electron lasers (XFEL) [1,2]. Correlation properties of the wave fields are calculated at different distances from an equivalent Gaussian Schell-model source. This model is used to describe coherence properties of the five meter undulator source at the synchrotron storage ring PETRA III. At a photon energy of 12 keV we estimated a transverse coherence of about 40 % in the vertical and about 1 % in the horizontal direction for both, high- and low-beta sections of PETRA III. Applicability of the Gaussian Shell-model has been analyzed for the same undulator length and different photon energies ranging from 3 keV to 20 keV. This analysis has shown that the Gaussian Schell-model can be effectively used for high photon energies above 6 keV. In the case of XFEL sources the decomposition of the statistical fields into a sum of independently propagating transverse modes is used for the analysis of the coherence properties of these new sources [1,3]. A detailed calculation is performed for the parameters of the SASE1 undulator at the European XFEL. A transverse coherence of about 60 % in the vertical as well as in the horizontal direction was obtained in the frame of the Gaussian Shell-model. It is demonstrated that only five modes contribute significantly to the total radiation field of that source. For a limited number of contributing modes this approach significantly simplifies numerical calculations of the correlation properties of the fields by reducing the number of variables. This may be especially important for the beam line characterization.

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[3] A. Singer, I. Vartanyants et. al. PRL 101, 254801 (2008)

Poster Number: 64

Coherence and wavefront characterization of Si-111 monochromators using double-grating interferometry

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The optical elements in a synchrotron beamline can drastically change the coherence properties of the x-ray beam by introducing vibrations and wavefront distortions. Several methods have been developed for the quantification of the coherence [1,2]. In many of these studies, a transverse coherence length smaller than expected is usually found. This is often attributed to vibrations or imperfections of the optical elements, without further experimental proof. Using a double-grating interferometer in the hard x-ray regime [3] we can measure both the complex coherence factor and the radius of curvature of the x-ray wavefront, which enables us to distinguish coherence degradation effects caused by vibrations of the optics from wavefront distortions caused by static imperfections [4]. In this work we compare the coherence and wavefront properties of an x-ray beam after a channel-cut monochoromator (CCM) to those after a double-crystal monochromator (DCM), both installed at the ID01 beamline at the European Synchrotron Radiation Facility (ESRF). When the DCM is used, our study reveals an effective source size in the vertical direction which is two times larger than expected, most likely due to relative vibrations between the two crystals. On the other hand, when using the CCM, a source size only slightly larger than expected is measured. Additionally, the wavefront distortions as a function of focusing with mirrors and with the bendable second crystal of the DCM are quantified. Our method is of relevance for the choice of optical elements for coherent diffraction experiments.

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Poster Number: 65

Coherence propagation – filtering properties of waveguides and mirrors

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New insights into many biological samples are possible with Coherent Diffractive Imaging (CDI): When absorption contrast is very low, scattering due to phase shifts is the only information we get. But a phase-sensitive experiment needs a coherent illumination: Otherwise no interference fringes can form, the phase-information is not available. With CDI, resolutions of down to 50 nm have been achieved recently [1,2]. In the times of 3rd generation synchrotron radiation sources and with the advent of the 4th generation (free electron lasers like the FLASH in Hamburg or the LCLS in Stanford) sources with a high brilliance and coherence are available. The high spatial degree of coherence is achieved by a small source size (10 to 100 μm) and a large distance from the source to the optics and samples (50 to 1000 m). We present numerical investigations on coherence propagation from the source to the sample with emphasis on coherence filtering by slits, mirrors and X-ray waveguides. All these three elements act as virtual sources and influence not only the divergence and intensity, but also the coherence properties of the X-ray beam. Our approach is based on stationary stochastic optical fields and ergodicity. The aim of this work is to optimize the optical elements in terms of coherent flux [3].

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[2] S. Kalbfleisch et al, SRI proceedings (2009) (accepted).
[3] M. Osterhoff, T. Salditt (in preparation).

Poster Number: 66

Coherence properties of the European XFEL

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The European x-ray free-electron laser (XFEL) will provide x-ray self-amplified spontaneous emission (SASE) FEL radiation in the wavelength range from below 0.1 to 3 nm using three undulator systems. The SASE mode of operation at the European XFEL defines specific behavior of longitudinal and transverse coherence properties. In this paper, we describe the evolution of the temporal and transverse correlation functions along the undulator length, and we extract the corresponding evolution of coherence time and degree of transverse coherence as typical figures of merit. Generation of coherent radiation inside the FEL undulators is followed by beam transport to the experiments. During transport, the total number of coherent modes is preserved, but the wavefront can be disturbed, and we analyze the conditions under which this occurs. It is emphasized that the development of experimental observables for the degree of coherence and wavefront properties will be important for experiments using coherent x-ray radiation.

Poster Number: 67

Design of the Imaging and Coherence Beamline I13L at Diamond

Dr. Ulrich Hilmar Wagner, Dr. Zoran Pesic, Prof. Christoph Rau

Diamond Light Source

Beamline I13L is a 250m long beamline currently under construction at the Diamond Light Source. The beamline consists of two different branches, one dedicated to imaging in direct and one dedicated to imaging in reciprocal space. The later branch will allow experiments requiring large lateral coherence length and well defined wave-fronts. This paper will discuss the optical layout of the beamline and operation modes of the beamline. Furthermore the impact of different optical components onto the coherence properties and will be discussed.

Poster Number: 68

Coherent X-ray Diffraction at Beamline I13L of Diamond Light Source

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I13L beamline is designed to fully exploit the brightness and flux provided by the Diamond storage ring for coherence based experiments [1-3]. The coherence length and the beam size and will be attuned by using variable focal length lenses and KB mirrors in order to match the size of the sample, ranging from submicron size up to 20-30 μm. The layout of the experimental setup will be presented. The experimental equipment shell provide possibility to pursuit speckles around the Bragg peak with a high-resolution detector (55 μm pixel size) positioned 0.1-5 meters from a sample, with the possibility to vary the azimuth (elevation) angle in the range 0-45 (0-60) degree. An attention is paid to optimize the stability of the detector arm to the micrometer scale. Moreover, an additional detector is planned to be commissioned for the ptychography experiments, positioned up to 20 m from the sample.

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Poster Number: 69

Hard X-ray delay line for correlation spectroscopy and pump - probe experiments at XFEL sources

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Probing matter on time scales ranging from typically several to nanoseconds is one of the key topics at X-ray Free Electron Laser (XFEL) sources. The accessible time windows are however compromised by the intrinsic time structure of the source. One way to overcome this limitation is the usage of delay line techniques. The prototype delay line device capable of splitting an X-ray pulse into two adjustable fractions and recombining them with the aim to perform X-ray Photon Correlation Spectroscopy and pump - probe type studies was designed and manufactured. Its performance has been tested with 8.39 keV and 12.4 keV X- rays at various synchrotron sources. The intrinsic throughput of the device at 8.39 keV is 0.6%. The stability was verified at 12.4 keV and found to be stable for at least 2 hours of operation. Time delays up to 2.95 ns has been achieved. The resolution of the applied time delay is limited by the delay unit diagnostics. The highest achieved resolution was 15.4 ps. The coherence properties of the X-ray beam passing through the delay line was investigated by a slit diffraction and static speckle pattern analysis. A high fringe visibility and a contrast of 56% was found, indicating a feasibility of performing coherence based experiments with the delay unit at XFEL sources.

Poster Number: 70

Table Top EUV/XUV Setup using a Nitrogen Plasma Source for Imaging and Spectroscopy

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The work on novel holographic and lens-less diffraction imaging techniques has potentials to overcome current limitations in X-ray microscopy. The aim is to decouple the achievable resolution from the current limitation in nanostructuring of X-ray lenses (e.g. Fresnel zone plates). Using a plasma-based soft X-ray source it is possible to investigate light-induced phenomena with a temporal resolution down to the sub-picosecond regime. In the short time laboratory of the Courant Research Center a laser-induced plasma in gas targets[1] (N, Kr, O) generating EUV/XUV radiation in the water window will be installed. In this energy regime, the investigation of biological samples (e.g. lipid-membrane systems) can be performed. Using an EUV/XUV source the experimental setup presented in this poster provide a wide range of experimental concepts. The compact experimental chamber can be operated both at a home laboratory source and as a synchrotron endstation. This allows users to study new methods and procedures at the laboratory source followed by experiments with higher resolution and source brilliance at the synchrotron. Building upon the optical bench and breadboard principles established in light optics, the setup allows one to arrange optical elements almost arbitrarily. The optical elements are mounted on standardized in-vacuum compact linear and rotational stages. Thus the modular principle of the whole setup allows the implementation of alternative targets, lasers or sources. Commissioning is planned to start in autumn 2010. Proposed experiments include • X-ray imaging (coherent diffractive imaging or zone plate based) • Scanning techniques (ptychography[2], STXM, etc.) • Waveguide optics[3] • In-line X-ray holography[3] • NEXAFS spectroscopy[4]

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Poster Number: 71

Ultrafast coherent imaging using UV-X harmonic beamline

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Coherent X-ray diffraction has demonstrated a very high potential in imaging single non periodic nanometer scale structures. Access to femtosecond dynamics relevant in major biological, physical or chemical processes requires obtaining single shot data. Up to now, this ability was limited to intense coherent pulses from a free electron laser. Laser-driven ultrashort X-ray sources offer a comparatively inexpensive and widely available alternative. In this work, using a table top high laser harmonic source optimized by using a soft X-ray wave front sensor, we demonstrate the capability of measuring diffraction patterns of nano-objects in single shot with an integration time of 20 femtoseconds. Images are reconstructed using a phase retrieval approach with a spatial resolution of 78 nm in single shot and 60 nm in multishots.

Poster Number: 72

Progress on coherent diffraction imaging at SPring-8 Compact SASE Source

Dr. Jaehyun Park, Dr. Changyong Song, Mr. Daewoong Nam, Dr. Yoshiki Kohmura, . Dr. Yonekura, Dr. Mitsuru Nagasono, Dr. MakinaYabashi, Prof. Tetsuya Ishikawa

RIKEN SPring-8 Center

The coherent diffraction imaging (CDI) technique has been widely used to study biological and material samples. High resolution imaging of biological specimens, however, has been deferred limited by radiation damages on the samples. As a prototype FEL source, SPring-8 Compact SASE Source (SCSS) has been constructed. SCSS provides EUV laser light of 50 ~ 60 nm wavelength and ~10^12 photons per pulse up to a 60Hz repetition rate. In this work, we could obtain the strong speckle patterns from nanostructures even for a single pulse. The speckle pattern has been changed as the radiation dose on the sample was increased by the series of the single pulses. It may directly show the proceeding of radiation damage on the sample and give some clues on the radiation damage effect for the high flux beam of XFEL.

Poster Number: 73

The Coherence Beamline P10 at PETRA III/DESY

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DESY

PETRA III, a high energy, high brilliance synchrotron at the DESY side in Hamburg was inaugurated at the end of 2009. Currently, it is the brightest storage ring based x-ray source with an achieved horizontal emittance of 1nm rad. A total of 14 undulator beamlines are either in the final construction phase or starting to operate [1]. The Coherence Beamline P10 is one of the first beamlines to start operating. P10 is designed to exploit the high brightness of PETRA III to provide and develop coherent x-ray scattering tools to investigate structure and dynamics on nanometer length scales. The two main experimental techniques will be X-ray Photon Correlation Spectroscopy (XPCS) and Coherent Diffraction Imaging (CDI). The beamline is equipped with a 5m undulator and its predicted coherent flux in the medium hard x-ray regime (5-15 keV) is expected to be significantly higher than at any other 3rd generation synchrotron source. Currently, the PETRA III synchrotron is operating at 50mA in top-up mode and first commissioning experiments have been performed at the P10 beamline. We will give an overview of the layout and the actual status of the Coherence Beamline and present first experimental results.

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Poster Number: 74

The Energy Recovery Linac: A Coherent, Hard X-ray Source

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Energy Recovery Linacs (ERLs) have potential to be superb, coherent, quasi-continuous, hard x-ray sources. ERLs are described, with reference to a 5 GeV ERL design being studied at Cornell University. Current progress at the Cornell ERL R initiative will be summarized. The properties of this ERL, and the x-ray beams that may be produced, are described and spectral curves are calculated and compared to other existing and future x-ray sources. ERLs will be especially advantageous in a variety of coherent and nanobeam experiments, especially where the sample must be repetitively probed due to the nature of the sample or the experiment. ERL strengths are elaborated relating to the very high coherent flux, inherently round beams, flexibility and quasi-continuous time structure of the sources. Examples are given where these x-ray characteristics will facilitate advancement of important "big challenge" areas of science.

Poster Number: 75

The holographic imaging setup at the P10 beamline of Petra III

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The upcoming x-ray source PETRA III at DESY/Hamburg (Germany) will provide outstanding coherence properties. This source will enable a novel quality of hard x-ray coherent imaging based on iterative and holographic object reconstruction. We are commissioning a dedicated setup for biological imaging at PETRAIII with optional cryogenic environment for biological samples, and in-situ optical microscopy. The beam path is based on a non-dispersive coherent focusing scheme, compatible with monochromatic and pink beam operations, and a wide range of coherent imaging modalities. A fixed curvature Kirckpatrick-Baez (KB) mirror system with EEM polished mirrors [1] will provide a focal spot of about 200 nm diameter. For further beam reduction and cleanup as well as for additional coherence filtering, an x-ray waveguide stage with a set of 2nd generation x-ray waveguides can be inserted in the focal plane [2,3,4]. Fresnel-type coherent diffraction imaging (fCDI) [5] as well as cone-beam holographic imaging based on an in-line (single beam) or off-axis (dual beam) configuration can be carried out [6]. All modalities can be extended by scanning [7] and tomography options, enabling large field of view in 3D. We will present first experimental results of waveguide-based x-ray microscopy and the coherence characteristics obtained with the setup at P10.

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Poster Number: 76

The new Diamond beamline I13L for Coherence and Imaging

Rau Christoph, Ulrich Wagner, Zoran Pesic

Diamond Light Source Ltd.

We present the project for the Coherence and Imaging beamline I13L at Diamond. Its purpose is to study Micro- and nano- structured materials from different scientific areas such as biomedicine, materials sciences, geo- or astrophysics. The beamline is designed to perform and promote high resolution imaging and tomography beyond today's limits. This goal can be achieved by imaging either in real or reciprocal space. For both methods two independent experimental stations will operate at a distance of about 250m from the source. On the 'imaging' branch in-line phase contrast imaging and microscopy with 1μm-50nm spatial resolution will be performed. The coherence' branch is foreseen for coherent diffraction imaging methods with resolution beyond the limits given by detectors and X-ray optics. We will present the different possibilities available at the new beamline as well as details about the challenges and innovations originated from this project.

Poster Number: 77

UHV Diffractometer for Coherent X-ray Scattering at Petra III

Mr. Marcel Buchholz, Mr. Chun-fu Chang, Mr. Christoph Trabant, Mr. Christian Schüßler-Langeheine

University of Cologne

Resonant scattering in the soft x-ray range is a powerful technique to study nano-scale order phenomena like charge, orbital and spin order in strongly correlated electron systems as well as magnetic properties of thin films, multilayers and other nanostructures. We are presently setting up a new UHV diffractometer for the XUV beamline of PETRA III in Hamburg. Because of the ultra-high brilliance of PETRA III, a high coherent flux can be expected. The instrument, equipped with an in-vacuum moveable CCD camera and pin-hole stages, is well suited for x-ray photon correlation spectroscopy (XPCS) experiments in the soft x-ray range. The XUV beamline with its energy range from 200 eV up to 3 keV covers the most important resonances of 3d, 4f and light 4d systems as well as of semiconductors, consisting of Zn, Ga, Ge, As and Se, and provides full polarization control. For the analysis of the scattered photons a polarization analyzer is available. The instrument is moveable and can also be used at FLASH. The scientific focus of our work is on systems, whose macroscopic properties are governed by the coexistence of different phases. One out of several prominent examples are the CMR-manganites, where STM-experiments found different coexisting domains of insulating and metallic character [1]. From the small switching field and from the observation that a certain amount of static disorder is required for the CMR effect [2] one concludes that the small external field may drive the system across the percolating threshold of the metallic regions rather than involving a phase transition of the whole sample. Similar effects are discussed also for other materials like high-Tc cuprates and are generally referred to as 'complexity' in solids [3]. Besides the fascinating nature of complexity in solids, phase separating materials also offer attractive technologically opportunities: macroscopic properties can be tuned by affecting only a small part of the sample, i.e., with small external fields. XPCS can be used to study disorder on different time and length scales in inhomogeneous materials and is therefore the ideal tool to study the relation between macroscopic properties and local electronic structure in such kind of systems. We report about our first XPCS experiments from complex materials at the 3rd-generation synchrotron radiation facilities BESSY II and ESRF. Funded by the BMBF through project 05KS7PK1 and by the DFG through SFB 608.

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