systems. The plastic strain distribution obtained in this way provides a general correlation between plastic deformation history and the properties of the observed diffraction peaks.

Keywords: strain scanning, synchrotron radiation, magnesium alloy

MS21.25.5

Acta Cryst. (2005). A**61**, C33

Depth-resolved Strain Measurements by Energy-variable X-ray Diffraction

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Characterization of the microstructure of materials with spatial resolution is one of key issues in materials related fields from nano-technology to non-destructive testing of manufactured articles. Depth resolved strain/stress measurements by diffraction methods are of particular interest. In order to improve depth resolution of x-ray diffraction, we are developing novel technique for synchrotron beam lines – energy-variable diffraction (EVD) [1]. The method is based on our ability to precisely change energy of synchrotron radiation and, in a result, to accurately control the x-ray penetration depth. Comprehensive analysis of x-ray trajectories, taking into account the instrument misalignment, change of the height of an incident x-ray beam with energy, and variable penetration of x-rays into the sample depth, allowed us to receive analytic expression for the diffraction profile measured by EVD and to show that the maximum diffraction intensity registered in the detector is coming from certain depth, which is energy-dependent [2]. This finding opens a way for measuring residual strains with high depth resolution by changing the x-ray energy in small enough steps.

Experimental examples taken with differently scaled metal/metal and metal/ceramic multilayers as well as structures from nature (seashells) demonstrate the capabilities of the method.

[1] Zolotoyabko E., Quintana J. P., *Rev. Sci. Instr.*, 2002, **73**, 1663. [2] Zolotoyabko E., Quintana J. P., *J. Appl. Cryst*.,2002, **35**, 594. [3] Zolotoyabko E., Quintana J. P., *Nucl. Instr. & Meth. B*, 2003, **200**, 382. [4] Zolotoyabko E., Pokroy B., Quintana J. P., *J. Synchr. Rad*.,2004, **11**, 309.

Keywords: residual strains, X-ray diffraction, multilayers

MS22 SINGLE PARTICLE X-RAY DIFFRACTION IMAGING

Chairpersons: Janos Hajdu, Henry Chapman

MS22.25.1

Acta Cryst. (2005). A**61**, C33

Diffraction Imaging of the Yeast Cell: First Results

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We have developed an apparatus for soft x-ray diffraction microscopy (XDM) of dry or frozen hydrated biological specimens. The microscope, stationed at beamline 9.0.1 of the Advanced Light Source, can collect nearly complete three-dimensional diffraction data to 10 nm resolution. Diffraction patterns, from eight angular orientations of a whole and unstained freeze-dried yeast cell, were recorded with the microscope and phased using the difference map algorithm. The resulting images portray the natural complex refractive contrast of the cell to 30 nm resolution and their agreement provides confidence in the accuracy of the imaging technique. New techniques for handling noisy and incomplete diffraction data were developed and improved the convergence of the algorithm. The effects of large doses on the structure of the cell were also investigated and it is determined that dry specimens suffer from shrinkage while frozen hydrated cells are stable with doses as large as 5×10^9 Gray.

Keywords: X-ray diffraction, X-ray imaging, X-ray microscope

MS22.25.2

Acta Cryst. (2005). A**61**, C33

Imaging Magnetic Nanostructures by X-ray Holography

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While holography has evolved to a powerful technique in the visible spectral range, it is difficult to apply at shorter wavelength as no intrinsically coherent (soft) x-ray laser is yet available as a light source. The progression from visible light towards shorter wavelength is motivated by the increase in spatial resolution that can be achieved. Of equal importance is the possibility to exploit special contrast mechanisms provided by scattering in resonance with transitions between electronic core and valence levels.

We demonstrate imaging of non-periodic objects by x-ray spectro-holography at 50 nm spatial resolution. Magnetic domain patterns forming in thin film Co-Pt multilayers with perpendicular anisotropy are imaged using x-ray magnetic circular dichroism contrast at 778 eV photon energy. The images are obtained by direct Fourier inversion of the coherent scattering pattern, without the need of phase retrieval or an iterative computing process. Holography at this wavelength was made possible by combining the sample with a nanostructured mask. [1] This approach is particularly valuable for future single shot and/or single molecule imaging experiments at free electron x-ray lasers. At such sources, the coherent x-ray flux will be sufficient to record a coherent x-ray diffraction snapshot using a single x-ray pulse with a duration of a few femtoseconds.

[1] Eisebitt S., Lüning J., Schlotter W. F., Lörgen M., Hellwig O., Eberhardt W., Stöhr J., *Nature*, 2004, **432**, 885.

Keywords: holography, coherent scattering, electronic structure and magnetism

MS22.25.3

Acta Cryst. (2005). A**61**, C33

Prospects for X-ray Diffraction Imaging of single Biological Molecules

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Short x-ray pulses from x-ray free electron lasers (XFELs) may enable diffraction imaging of single biological molecules. This would allow the determination of the structure of many molecules that have, to date, resisted crystallization. Since the appropriate sources will not be available for a few years, experimental design currently has to be done through simulations and modeling. Various aspects of the models are tested through experiments on currently available light sources.

In this presentation we will discuss numerous issues of the injection, irradiation, and imaging process. We will present our plans to model all aspects of the diffraction imaging endeavor, and the progress that we have made to date. Specifically, we will present an analysis of the pulse length and photon energy requirements by combining results from a continuum damage model [1] with a fluence requirement model [2]. We will further discuss several means to alleviate the pulse requirements, and compare the requirements with parameters of two planned x-ray lasers. Finally, we will present results from recent 3D imaging experiments at a resolution down to 10nm.

[1] Hau-Riege S.P., London R.A., Szoke A., *Phys. Rev. E*, 2004, **69**, 051906. [2] Huldt G., Szoke A., Hajdu J., *J. Struct. Biol.*, 2003, **144**, 219.

Keywords: diffraction imaging of non-crystalline specimens, biological molecules, radiation damage studies

MS22.25.4

Acta Cryst. (2005). A**61**, C33-C34

Imaging of Atom Clusters by hard X-ray free Electron Laser Pulses

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We study the possibility of imaging a small cluster of atoms by

short x-ray free electron laser pulses. A special molecular dynamics model has been developed to describe the Coulomb explosion of the clusters [1]. We use numerical modeling based on the non-relativistic classical equation of motion. Quantum processes are taken into account by the respective cross sections. The explosion dynamics is examined for various conditions: pulse length, constituent atomic number, number of photons in a pulse. We use our model to get an estimate of the time available for imaging before the cluster deteriorates significantly. Based on these results we calculate the continuous elastic scattering pattern of the sample and try to reconstruct the original atomic order from this pattern. We use a density modification type algorithm analogous to the Fienup hybrid input output reconstruction method [2,3]. Since this method needs a 3D dataset in the reciporocal space, scattering patterns have to be taken at various sample orientations. That requirement leads to a multi shot experiment. Therefore the full dataset have to be built from scattering patterns of several independent exploding clusters. We included this complication in the calculations. We found that the shorter the pulse the higher the ratio of the photons useable for imaging. The conclusion of the calculations is that the pulse length of the presently planed x-ray free electron lasers is too long.

[1] Jurek Z., Faigel G., Tegze M., *European Physical Journal D*, 2004, **29**, 217. [2] Fienup J.R., *Optics Letters*, 1978, **3**, 27. [3] Jurek Z., Oszlanyi G., Faigel G., *Europhysics Letters*, 2004, **65**, 491.

Keywords: X-ray free-electron lasers, clusters, molecular dynamics simulations

MS22.25.5

Acta Cryst. (2005). A**61**, C34

Three-dimensional Data merging of Randomly Oriented Continuous Diffraction Patterns

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We have developed methods for the assembly of three-dimensional diffraction data from noisy and randomly oriented continuous diffraction images. Before a structural reconstruction is possible, the patterns must be oriented with respect to each other and the signal to noise ratio must be increased by averaging of redundant data. While certain aspects of this problem are similar to problems in single-particle electron tomography, there are also significant differences. In single-particle electron tomography, similar images are located based on their correlation and the mutual orientation of the averaged images is determined from the common lines of intersection of their Fourier transforms. We present an extension of this scheme to the case of diffraction images, which intersect in spherical sections in Fourier space rather than in planar sections and which have statistical properties different from those of tomograms. We study how our scheme works on both real and simulated sets of three-dimensional data.

Keywords: three dimensional image, imaging, fourier transform

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MS23 PUTTING THE PEDAL TO THE METAL: SPEEDING UP BIOLOGICAL STRUCTURE DETERMINATION

Chairpersons: E. Yvonne Jones, Peer R. Mittl

MS23.25.1

Acta Cryst. (2005). A**61**, C34

Development of a High-throughput Structure Determination Pipeline at BM14

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The basic operations to be performed for the collection of MAD and SAD data from protein crystals are well established and have been implemented successfully at beamlines across the world. There is now, however, intense activity aimed at revolutionizing the possibilities via a series of improvements, centered around (i) the mechanical aspects of automation, improved precision and improved visualization and (ii) the software aspects of automation and integration.

BM14 is a tunable bending magnet beamline at the ESRF operated by the UK research councils in collaboration with the EMBL Grenoble outstation. A high-throughput pipeline for structure determination by SAD and MAD phasing is being developed through our participation in the BBSRC e-science project e-HTPX (www.e-htpx.ac.uk).

An overview of the hardware and software implemented at BM14 for automation of macromolecular data collection will be presented. In particular, software developments which allow the user to keep track of the sample from their home lab to and from the beamline, as well as management of experimental data acquired, through the development of an easy to use beamline Laboratory Information Management System (LIMS) will be described. Our experiences in the use of SAD phasing with naturally occurring light atoms, such as sulphur and manganese, and their application for use in a high-throughput structure determination pipeline are summarized.

Keywords: MAD phasing, automation, LIMS

MS23.25.2

Acta Cryst. (2005). A**61**, C34

Automating Crystallographic Structure Determination Calculations

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Structural genomics efforts require a high throughput at all stages of the structure determination process. Simultaneously, it is important to reduce the cost per structure, which means reducing the time spent on each structure. We have focused on the structure determination calculations going from processed, merged data through to initial model. The Automated Crystallography System (ACrS) utilizes existing software and algorithms but a distributive program interface administers the programs for determining protein structures. A relational data base stores initial data for starting the process as well as harvesting and warehousing data generated during the structure determination process.

The ACrS default mode of operation is to try several defined pathways in parallel. Analysis of the results in the database provides information for improving the pathways and for selecting software with complementary strengths.

An example is a recently determined structure of a member of the ROK family of transcription regulators that used a “native” data set and SAD phasing from one bound zinc to automatically built 384 residues of 405 without any intervention or optimization of parameters.

Keywords: structural genomics, automatic structure solution, macromolecular structure

MS23.25.3

Acta Cryst. (2005). A**61**, C34-C35

HT Structure Determination at SER-CAT: Five Structures in 23 Hours

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Researchers at the University of Georgia (UGA) have developed an optimizing, high throughput structure determination pipeline (SCA2Structure) capable of providing fitted or partially refined structures in a matter of hours from anomalous scattering (MAD or SAD) data [1]. This powerful structure determination engine coupled with the excellent data collection facilities provided by the SER-CAT, beamlines at the Advanced Photon Source (www.ser-cat.org) provides the basis for high-throughput structure determination.

Using prescreened crystals and data collected at SER-CAT, UGA researchers were able to determine five SAS structures on-site during a recent 24-hour run. Data were processed at SER-CAT and input to