Development of coherent scattering and diffractive imaging and the COSMIC facility at the Advanced Light Source

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Abstract. A new facility is described that is being constructed for coherent scattering and microscopy at the Advanced Light Source. The undulator beamline delivers maximum coherent flux to two experiment programs. One is for soft x-ray coherent scattering and correlation studies, the other is for soft x-ray diffractive imaging using ptychographic reconstruction techniques. The energy resolution is sufficient for NEXAFS spectroscopy with full polarization control, from below the carbon edge to 2500eV. New instrumentation is planned for wavelength limited 2D imaging and 3D imaging at spatial resolution better than 10nm and for coherent scattering studies with a variety of sample environments including strong magnetic fields and cryogenic temperatures. High speed CCD detectors will make optimum use of the available flux on dedicated data transmission networks.

1. Introduction
Coherent x-rays are used in a scattering geometry for correlation studies of fluctuations in materials science. They also provide reconstructive imaging at spatial resolution several times better than that of lens-based x-ray imaging systems limited to a resolution of order 10nm. The development of these techniques into the soft x-ray regime [1,2] provides an additional spectroscopic capability by which certain species in compounds can be studied through resonant scattering or by absorption contrast. With control of the polarization of the soft x-ray beam, measurements can be made specific to certain magnetization states or to the orientation of chemical bonds. All these capabilities will be provided at COSMIC which is being constructed at the ALS now, through 2013.

2. Performance of the Facility
Several design options exist for a modern soft x-ray undulator beamline. VLS gratings can provide focusing in the dispersive plane and can reduce the number of reflections required [3]. Spherical grating monochromators can be employed in a horizontally dispersing paraxial geometry to provide convenient trade-off between resolution and coherent flux [4]. However, a major concern at the ALS is placement of the experiment stations and we have adopted a collimated PGM design [5]. Figure 1. shows the layout. The collimated section of the beamline is arbitrarily long, allowing for good separation of the experiments. Two plane gratings are required, with constant line density, 100 and 300 lines/mm. Coarse gratings at shallow angles provide high efficiency to 2500eV. The resolution is
modest (R≈2500) to maximize the coherent flux, and is not degraded by the thermal deformations of the optics. We have the flexibility to operate with good suppression of higher order light and the beamline can operate in zero order with the full source bandwidth. The source is a 36mm period elliptically polarizing undulator operating from 260eV through the C, N and O edges, covering the L edges of light elements and extending up to 2500eV which is optimum for high resolution diffractive imaging. The undulator provides complete polarization control. The source is diffraction limited in the vertical direction up to about 350eV. At higher energies, and in the horizontal direction, the principle rejection of incoherent modes is at the exit slit aperture. To provide stability of the illumination wavefront the cylindrical and toroidal mirrors will servo-steer horizontally through the exit slit to eliminate pointing drift. A second level of servo steering is provided in both directions by a toroidal relay mirror to the scattering pinhole, and this mirror is lighter, so there is a possibility of a higher speed loop working to reduce the effect of vibrations.

Figure 1. Schematic beamline layout illustrating component function.

Figure 2. shows the computed coherent flux (photons/second) at the imaging zone plate lens. Curves are shown for each grating at different values of \( C = \cos \beta / \cos \alpha \). \( C \) can be tuned. Higher values of \( C \) give higher spectral resolution and extended range. Lower values give higher efficiency and better suppression of higher order light. The dashed curves show the flux in third order diffraction at three times the photon energy. When ALS installs new sextupoles in 2013 the source brightness and coherent flux will be increased by about a factor three.

Figure 2. Computed coherent flux in various operational modes, into \( \lambda^2/4 \) phase space with a resolving power approximately \( R=3,000 \).

3. Instrumentation for scattering

Coherent x-ray scattering allows us to undertake time dependent studies of equilibrium fluctuation, which is the x-ray analog of the photon correlation spectroscopy. Diffuse scattering due to coherent x-rays give rise to speckles due to the interference of scattered wave fronts that are randomly phase shifted by the morphology of the sample. For magnetic system the use of resonantly tuned coherent x-
ray gives magnetic speckles which are representative of the exact lateral magnetic heterogeneity. Any change in the surface morphology causes a subsequent change in the speckle pattern. By monitoring the speckle pattern over time at a particular temperature and/or field it is possible to determine the temporal evolution of the surface features such as domain. Fig. 3 shows a speckle pattern obtained at the Co L$_1$ edge is shown. The sample used was 6 monolayers of Co on 2 monolayers of Au and the sample exhibits spin reorientation transition. The speckle pattern contains both charge as well as magnetic speckle. A time series of speckle pattern was measured as a function of temperature from which the dynamic structure factor was evaluated. [1]

Coherent x-ray scattering could also be used to perform speckle metrology measurements and obtain unique information not possible with partially coherent beams. For example, it is possible to obtain information about spatial symmetries by calculating angular correlation of a speckle pattern. We have recently performed similar experiment on Co/Pd/ItMn system and showed existence of hidden symmetries [2]. While these types of measurements are routinely done at the ALS, the new COSMIC facility will provide coherent photons 2 orders of magnitude higher in a narrower bandwidth. Thus faster time scales (several microseconds) will be possible to access. The new facility will also provide circularly polarized x-ray beam which will enable us to perform polarization dependent studies over a wide range of soft and hard condensed matter, a feature which is absent at the moment.

4. Instrumentation for imaging

Figure 4 R+D efforts for the development of ptychography at the ALS. (a) The Nanosurveyor instrument with cryo-sample rotation stage and interferometer position sensing. (b) and (c) show the ptychographic reconstruction and a STXM image of a zone plate with 20 nm lines respectively. The STXM image was generated using a 25 nm outer zone width focusing optic while the ptychographic data was generated using a 60 nm optic. Both images have 5 nm pixel size and display the x-ray intensity. The scale bar is 200 nm.

An R+D effort is underway to develop a microscope suitable for ptychographic tomography with soft x-rays on samples in vacuum that can be measured at high or low temperatures. This instrument is NANOSURVEYOR and is a prototype for the imaging microscope at COSMIC. A zone plate forms a coherent illumination spot of the order 300nm diameter on the sample and diffraction patterns are
recorded, along with accurately encoded values of the sample position, as the sample scans in x and y over a region of interest of the order 10 microns. The redundancy required for robust numerical reconstructions is provided by overlapping the illumination between successive exposures. The sample position encoding is critical. Inaccurate sample placement is tolerable if the position is measured. A novel differential interferometer scheme is employed measuring the zone plate lens with respect to the sample in x and y, reflecting one of the x beams from a cylindrical sample chuck through a cylindrical lens. Sample encoding within an x/y scan is accurate to about 10nm. Ptychographic images will be reconstructed in this way at each orientation for tomography, with transverse registration between views to about 300nm, limited by the precision of the sample chuck. This R+D program will inform the choice of optimum illumination geometry and detector pixellation, along with the most effective scan scheme. Other development experiments are underway utilizing the ALS STXM at beamline 11.0.2 which has been retrofitted with a CCD camera and which are optimized for spectro-microscopy. Figure 4 shows a CAD drawing of the NANOSURVEYOR instrument and a demonstration of the current imaging capable using a STXM enhanced with ptychography at 800eV x-ray energy.

5. Detectors

A large detector dynamic range is required for these experiments because the scattered intensity drops rapidly (~q^-4) with angle and there is an un-scattered bright field containing important information about the large scale structure of the image. Photon collecting CCDs are the best option, with useful efficiency in the soft x-ray regime. To increase speed, we have developed a design capable of 200 frames/sec, 15 bits dynamic range with a 12 bit ADC and 1M pixels, called 1kFSCCD This is soon to be replaced by a 1000 frames/sec column parallel camera. These detectors [6] have 100% quantum efficiency and can collect 360 photons per pixel at 1keV. The dynamic range is extended by making multiple exposures, as many as about ten per x/y position. The 1kFSCCD camera head produces a continuous stream of raw data at a rate of about 400 MB/s. To keep up with this large data rate and to prepare for the next generation column parallel camera a scalable CCD readout system has been developed based on the PICMG 3.1 Advanced Telecommunications Computing Architecture (ATCA) specification [7]. The 1kFSCCD camera readout system deviates from this with the removal of the redundancy requirement in order to double the available bandwidth on the backplane and with stripped down implementations of standard Ethernet protocols developed in firmware, further expanding its capability of handling fast detectors.

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6. References

[1] K. A. Seu, S. Roy, J. J. Turner, S. Park, C. M. Falco and S. D. Kevan, Phys. Rev. B. 82, 012404 (2010).
[2] R. Su, K. A. Seu, D. Parks, J. Kan, E.E. Fullertion, S. Roy, and S. D. Kevan, Phys. Rev. Lett.107, 257204 (2011).
[3] Reininger, R., Kriesel, K., Hulbert, S.L., Sanchez-Hanke, C. and Arena, D.A., Rev. Sci. Instrum.,79, 033108 2008
[4] Warwick T., Ade, H., Kilcoyne, K., Kritscher, M., Tyliszczak, T., Fakra, F., Hitchcock, A., Hitchcock, P. and Padmore, H., J. Synchrotron Rad. 9 (2002) 254-257
[5] Follath, R., and Senf, F., Nucl.Instrum. Methods Phys. Res. A390 (1997) 388
[6] Denes,P.,Doering,D.,Padmore,H.A.P.Walder,J.-P.,and Weizeorick,J.,Rev.Sci.Instrum. 80 (2009) 083302
[7] D. Doering, et al. Nuclear Science Symposium and Medical Imaging Conference (NSS/MIC), 2011 IEEE , pp.1840-1845, 23-29 Oct. 2011