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Possibilities at the Polar beamline with APS-U

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Abstract. The Polar beamline will make use of the small emittance of the new APS-U storage ring and will offer extremely brilliant and coherent beam of variable polarization in the hard x-ray range. Tailored optics and experimental equipment will enable high spatial resolution dichroic spectroscopy, reflectivity and diffraction in combination with extreme pressures, low temperatures and high magnetic fields. Dichroic direct and ptychographic imaging of magnetic structures is being developed and will make use of the largely enhanced coherence of the low emittance source. We present an overview of the planned instrumentation and the upcoming new exciting possibilities.

1. Introduction

Nanoscale electronic and structural inhomogeneities are prevalent in condensed matter physics. Whether a result of competing ground states in correlated electron systems, such as charge density waves and superconductivity in high-Tc materials or driven by the energetics of domain and vortex wall formation in magnetic and ferroelectric systems, nanoscale inhomogeneity plays a key role in dictating emergent properties of functional materials. To unravel the connection between nanoscale inhomogeneity and emergent properties, polarization dependent resonant x-ray spectroscopy and scattering methods with element- and orbital-selectivity are crucial.

In 2024, the upgrade of the Advanced Photon Source (APS-U) at Argonne National Laboratory to a multi-bent-achromat (MBA) reverse bent lattice will be completed. APS-U will offer extremely brilliant and highly coherent beam through the new low emittance source [1] to the user community. This will enable a variety of exciting new possibilities for dichroic scattering and spectroscopy experiments by pushing towards extreme pressures and high spatial resolution. Polar, the beamline for polarization modulation spectroscopy at sector 4 of the APS will make use of these new possibilities in terms of small focus sizes, coherence and polarization.

New Superconducting Arbitrarily Polarizing Emitter (SCAPE) undulators [2] which are being developed for the Polar beamline will make accessible especially the energy range above 14 keV for magnetic spectroscopy experiments. Energies above 14 keV are normally not reachable at conventional hard-x-ray beamlines using phase plates for polarization manipulation, and will enable investigation of magnetic properties of materials at the 5f L- and 4d K-edges using spectroscopic methods. The hard x-ray regime is particularly attractive for high-pressure experiments as the diamond anvils become x-ray transparent. In addition to these new capabilities for photon energies above 14 keV, the new SCAPE undulators will also provide increased polarized flux at the energies down to 2.75 keV, as shown in Fig. 1 left. Small focused and coherent beams down to 100 nm will allow reaching new areas in terms of resolution, by employing direct imaging or ptychographic methods, at low temperature, high magnetic fields and high pressures. Beamline optics will be designed to reduce vibrations to guarantee small focus sizes.

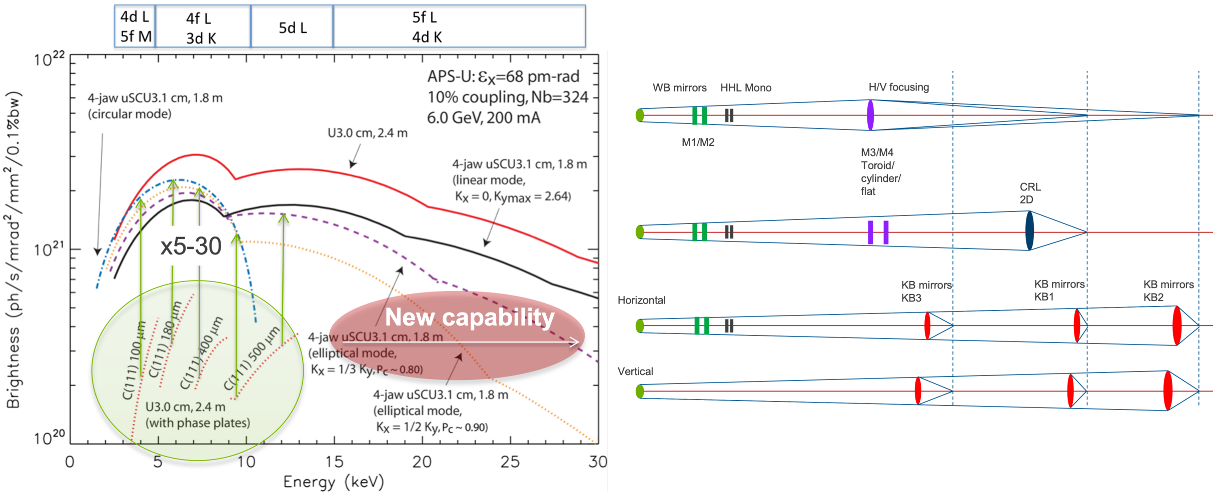

Figure 1. Left: Undulator spectrum of the SCAPE undulator (4-jaw uSCU3) for linear and circular mode and elliptical modes with different degrees of circular polarization (Pc), compared to the conventional linearly polarized undulator (U3.0). In the energy range below 14 keV, the expected flux increase of circularly polarized beam by up to one order of magnitude is shown by green arrows. Right: Focusing schemes for the two instrument locations with focus sizes shown in Table 1. Toroidal mirrors will be removed for KB and CRL focusing.

The two main experimental setups located in the two experimental enclosures 4-ID-G and 4-ID-H will make use of this new source and will allow polarization dependent scattering as well as absorption spectroscopy experiments covering all relevant absorption edges.

A low vibration, large bore superconducting magnet with 9 T longitudinal and 1 T horizontal and vertical transversal fields will allow X-ray magnet circular (XMCD) and linear dichroism (XMLD) measurements at extreme pressures using the sub-micron beam focused by the Kirkpatrick-Baez (KB) optics. A horizontally diffracting diffractometer with open chi circle and warm bore 2 T superconducting magnet will allow dichroic diffraction and spectroscopy experiments in moderate fields and at high pressures. An interchangeable high-precision sample stage will allow for dichroic imaging experiments using highly focused beam. These exciting new capabilities will contribute to the discovery of novel electronic states of matter at extreme pressure conditions and allow imaging electronic and magnetic inhomogeneities in quantum materials with tens of nanometer resolution. Especially the small source size of APS-U in combination with variable polarization will enable experiments currently not possible. Small focus sizes will allow to conduct experiments at extreme pressures of up to 6 Mbar using a diamond anvil cell (DAC) with double stage or toroidal anvils [3, 4]. This will allow to contribute to exploring properties of hydrides and sulfides in the quest towards room temperature superconductivity or to explore magnetism or mixed-valence superconductivity in lanthanides and actinides. The 100 nm focused beam at the diffractometer will allow direct imaging of magnetic and electronic domains as well as their evolution inside a DAC or in a strain cell.

The availability of both, increased coherence and variable polarization in the full energy range will open up exciting new possibilities for investigating magnetic, orbital and electronic order using dichroic ptychography as well as dichroic ptychographic tomography. Magnetic tomography has been demonstrated at the Swiss Light Source, using high dichroic contrast Gd L-edge resonance [5, 6]. Experiments will be possible with high spatial resolution allowing for example for spatially resolved mapping of magnetic, multiferroic or ferro-electric domains [7, 8].

2. Source

Fast polarization flipping between left and right circular as well as between horizontal and vertical linear polarization in the energy range from 2.7 to 27 keV will be possible with the new Superconducting Arbitrarily Polarizing Emitter (SCAPE) undulators which are currently being designed for the Polar beamline [2]. This will be achieved with the use of two in-line SCAPE undulators set to deliver horizontal and linear polarization (or circular left and right), respectively, and using small orbit bumps (30 urad) of the electron beam at frequencies up to 10 Hz to alternate polarization [9]. Storage ring orbit feedback, in combination with x-ray beam position monitors near focusing elements, are specified to maintain focused beam position with an accuracy of 10% of source size.

3. Optics

The first optical component in the first optical enclosure (4-ID-A) will be a pair of horizontally deflecting water-cooled white/pink beam (WB) mirrors (Fig. 2) used for heat load reduction for the subsequent vertical liquid nitrogen cooled double-crystal monochromator (VDCM). One of the mirrors is bendable to compensate for the defocusing effect of the heat bump at the first crystal of the VDCM. The VDCM from CINEL is specified to have relative and absolute angle stability of 50 nrad (RMS). It consists of a pair of side cooled Si crystals in the 111 Bragg reflection geometry ($d = 3.135$ Å), and a pair of 6H-SiC crystals in the 0006 Bragg reflection geometry ($d = 2.522$ Å), mounted on the cooled cooper blocks. This combination will allow preserving a high degree of polarization in polarized beams produced by the SCAPE undulators in the whole energy range from 2.75 to 27 keV. Vibration is reduced by having a larger first crystal with no degrees of freedom apart from the Bragg angle for energy tuning and on which the beam walks when energy is changed. The second crystal is small and lightweight with pitch and roll coarse and fine degrees of freedom at the crystal stage for horizontal and vertical beam position feedback.

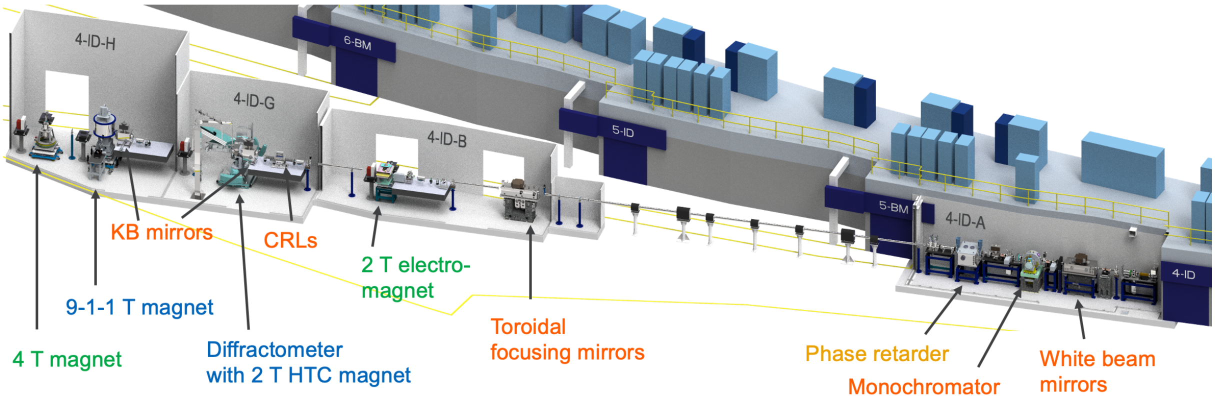

Figure 2. Polar beamline layout with first optical enclosure (4-ID-A) on the right housing the white beam mirrors and monochromator followed by the experimental stations 4-ID-B, 4-ID-G and 4-ID-H. Red labeled devices are new optical components and blue devices are new instruments. Orange and green devices are existing optics and instruments, respectively.

Table 1. Calculated flux and focal spot sizes in 4-ID-G and 4-ID-H for the different focusing optics using a 20x20 micro-rad^2 beam acceptance.

Enclosure	Mode	Energy	Focusing optic	Flux	Focal size
4-ID-G	high brightness	10 keV	K-B	1.3×10^{13}	114×92 nm^2
4-ID-G	coherent	10 keV	K-B + slit	1.6×10^{12}	200×200 nm^2
4-ID-G	medium spot	10 keV	CRL	1.1×10^{13}	2.0×0.9 μm^2
4-ID-G	large spot	10 keV	Toroids	2.4×10^{13}	32×4.1 μm^2
4-ID-H	high brightness	10 keV	K-B	2.1×10^{13}	414×212 nm^2
4-ID-H	coherent	10 keV	K-B + slit	1.4×10^{12}	790×560 nm^2
4-ID-H	large spot	10 keV	Toroids	2.6×10^{13}	35×5.9 μm^2

An existing phase retarder setup will be positioned downstream of the VDCM. Various optics will be available to provide different focus sizes (Fig. 1 right). Toroidal focusing mirrors in horizontal geometry will be located in 4-ID-B and allow focusing to both experimental setups with focus sizes of about 20 μm. Together with the WB mirrors they also provide suppression of higher order harmonics emitted by the insertion device in the whole energy range of Polar. The first mirror can be bent along its meridional direction. It has one Pd-coated sagittal cylinder and two flat regions, bare Si and Pt-coated, respectively. The second mirror, instead, has one Pd-coated flat region and two sagittal cylinders, bare Si and Pt-coated, respectively. KB-mirrors with working distances of 100 mm and 600 mm in 4-ID-G and 4-ID-H, respectively, will allow sub-micron focusing of 100 nm and 300 nm, respectively, as shown in Table 1. A transfocator housing parabolic Be lenses in 4-ID-G will provide intermediate focus sizes of 1-2 μm.

4. Beam conditioning and monitoring

Beam position will be controlled using horizontal and vertical feedback between XBPMs, installed upstream of each focusing optics (Toroidal and KB mirrors), and piezo actuators on the second crystal stage of the VDCM. An in-line rotatable polarimeter will allow full polarization characterization and control to characterize and monitor the degree of polarization provided by the SCAPE undulators. A chopper will be available for background subtraction for dichroic spectroscopy to achieve highest quality absorption spectra.

5. Experimental setups

Experiments will be located in two new enclosures with a diffractometer in the upstream enclosure (4-ID-G) and a high field magnet in the downstream enclosure (4-ID-H). The experiments will be operated alternatively with the possibility to access 4-ID-H for experiment preparation and magnet cooling and maintenance during experiments in 4-ID-G.

5.1. Diffractometer

A diffractometer for horizontal scattering [10] will be located in 4-ID-G. The omitted vertical sample rotation makes it a horizontal diffractometer with the advantage of allowing more space for sample environments. There will be two configurations of the sample goniometer that can be swapped above the horizontal base theta rotation. The first one is a Eulerian cradle with an open chi circle allowing unlimited angular access in the horizontal plane. A custom designed 2 T High-Tc superconducting magnet can be mounted in different geometries on the base sample rotation inside the Eulerian cradle as shown in Fig. 3 left and center. The 60 mm gap between

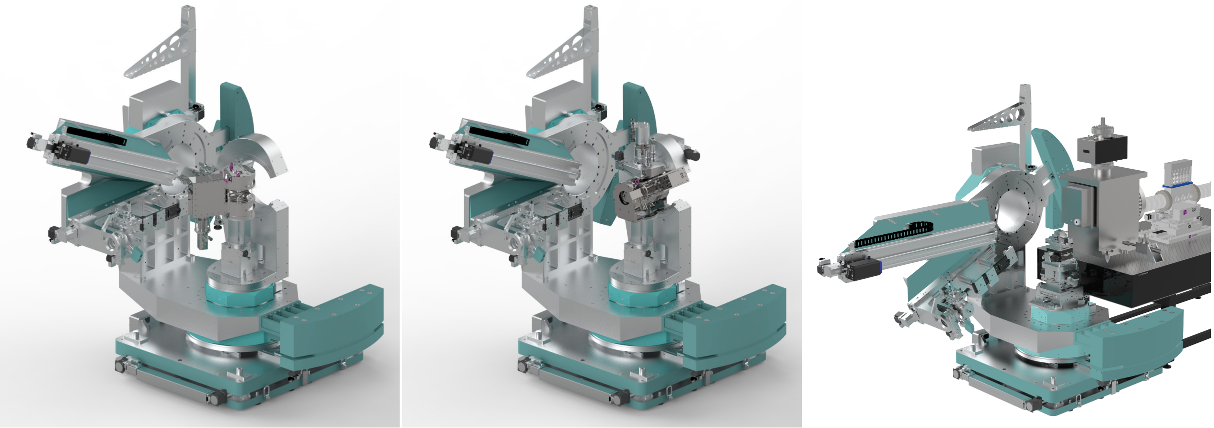

Figure 3. Diffractometer with (left) open Eulerian cradle and 2 T magnet in diffraction geometry with vertical field, (center) open Eulerian cradle and 2 T magnet in spectroscopy geometry with magnetic field along the beam and (right) interchangeable high precision goniometer with KB mirror tank and transfocator.

magnet poles allows usage of strain cells and mini-DACs mounted in sample cryostats that can be inserted in the warm bore area of the magnet using the Eulerian cradle. For the second configuration, the Eulerian cradle can be exchanged with a high precision setup consisting of a double tilt and a xyz-translation with a high-precision air bearing rotation on top, followed by a tilt, another xy-stage and a nano-positioner (Fig. 3 right). This setup will be used for 2D and 3D direct and ptyochographic dichroic imaging as well as Bragg coherent diffraction imaging (CDI) together with the KB mirror directly upstream of the setup. The horizontal and vertical detector rotations still provide access to out of plane reflections using either the 2D detector mounted on a 2 m arm or the point detector with optional in-vacuum polarization analyzer.

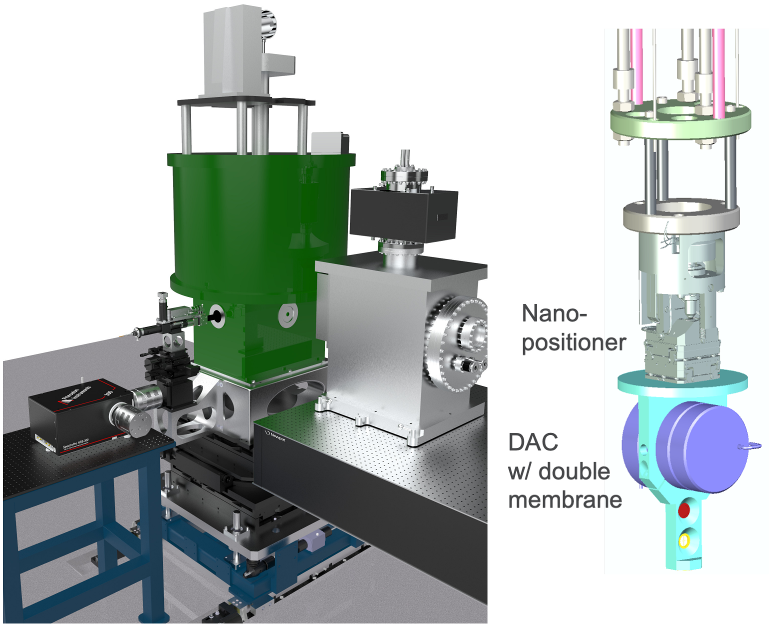

Figure 4. Left: 9-1-1 T magnet with KB mirror upstream and Raman system outboard. Right: Tip of probe with nano-positioner and double membrane DAC. Diagnostics for beam focus optimization as well as retroreflector mirrors are included in the DAC holder.

5.2. 9-1-1 T magnet

The large bore, low vibration 9-1-1 T magnet from Cryogenic Ltd., UK, will be located in 4-ID-H on top of a heavy load, high-precision positioning stage. Use of cryogenics for cooling the magnet cryostat instead of a cryogen free system was chosen to reduce sample vibrations to a minimum as it will be used for extreme pressure and domain imaging experiments making use of the 300 nm beam provided by the KB mirrors. The probe will be equipped with a nano-positioner inside the large bore 74 mm diameter variable temperature insert (VTI) and will allow mounting of DACs with compression and decompression membranes as well as strain cells for in-situ experiments. Interferometers will be monitoring for any vertical and horizontal sample displacements perpendicular to the x-ray beam which will be compensated with the nanopositioners. Re-entrant room temperature bores along the split of the horizontal field coils are equipped with Be and optical windows for use with a multi-element fluorescence detector and a Raman spectrometer, respectively. Beam diagnostics and retroreflector mirrors are mounted on the DAC holder for focus optimization and interferometry, respectively, as shown in Fig. 4.

6. Summary and Outlook

The Polar beamline will expand the frontier of dichroic x-ray studies in the hard x-ray regime by leveraging the increased brightness of APS-U as well as latest developments in superconducting undulator technology, x-ray optics, and high precision end-station instrumentation. High-flux-density, sub-micron beams with tunable polarization will allow exploration of electronic matter at extreme pressure as well as electronic texture at the nanoscale with ptychographic methods. The availability of low-temperature, high magnetic field, pressure, and uniaxial strain sample environments should allow for detailed exploration of electronic phase diagrams particularly in quantum materials relevant to information and energy technologies.

7. Acknowledgement

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