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Soft x-ray spectroscopy undulator beamline at the Advanced Photon Source

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ABSTRACT

Construction of the high-resolution soft x-ray spectroscopy undulator beamline, 2ID-C, at the Advanced Photon Source (APS) has been completed. The beamline, one of two soft x-ray beamlines at the APS, will cover the photon energy range from 500 to 3000 eV, with a maximum resolving power between 7,000 and 14,000. The optical design is based on a spherical grating monochromator (SGM) giving both high resolution and high flux throughput. Photon flux is calculated to be approximately 10^{12} - 10^{13} photons per second with a beam size of approximately 1 x 1 mm^2 at the sample.

1. INTRODUCTION

The driving force of the soft x-ray spectroscopy program at the Advanced Photon Source (APS) is to cover the soft x-ray photon energy range from 0.5 to 3 keV with a beam brilliance at the sample comparable to that of a typical Advanced Light Source (ALS) undulator beamline operating below 1 keV. The beamline uses a high-brilliance soft x-ray undulator source so that both high resolution (resolving power ~10^4) and high throughput can be achieved simultaneously. In addition, because it is based on a grazing-incidence geometry, the source polarization of the beam will be maintained at the sample. This will enable us to make use of a circularly polarized undulator at a later date. Our aim has been to construct a highly versatile beamline for spectroscopic studies of advanced materials, comparable to those found at the ALS, but with an operational energy from 0.5 keV up to the lowest operational energy of the standard APS undulator A at approximately 3 keV.

The soft x-ray (SXR) spectroscopy experimental program will be situated on branchline C of the sector 2 insertion-device port of the APS. Two undulators are installed in the sector 2 straight section: undulator A which is used for hard x-ray imaging/coherence-related experiments on beamline 2ID-D, and a custom 5.5-cm-period soft x-ray undulator, which has recently been installed for the spectroscopy beamline 2ID-C and the soft x-ray imaging/coherence beamline 2ID-B.[1] The 2ID-D and 2ID-B branchlines will not considered futher in this manuscript. The period of the SXR undulator was specifically chosen to reach a minimum energy of 500 eV, which will allow us to cover the important O 1s, Cu 2p, and 3d transition metal L edges. A summary of SXR undulator parameters is given in table 1, and the brilliance of the soft x-ray undulator and undulator A are shown in figure 1. In the future, we will move the 2ID-C spectroscopy branchline to sector 4, where a circularly polarized x-ray undulator will be installed. This device is based on a fully electromagnetic magnetic lattice, which is in the final stages of design. Fabrication of parts has already begun.

2. BEAMLINE LAYOUT

Manipulation of beam polarization with multilayers or crystals has not been achieved in the 1 - 2 keV region to date. Also, calculations indicate that, at best, phase shifts of a few degrees will be achievable.[2] We ultimately plan to use a variably polarized source together with a polarization-preserving monochromator. Initially we will be using a plane-polarized undulator source, and, in approximately two years the SXR spectroscopy program will be moved to sector 4, where a circularly polarized undulator will be installed. To preserve source polarization, we opted for a grazing-incidence spherical grating monochromator (SGM), to achieve high resolution.[3-6] At the same time, we decided to limit the upper range of the monochromator to 3 keV, since the majority of the scientific program is contained in this energy region, and a double-crystal, e.g., Si(111), monochromator has both higher efficiency and resolving power above 2.5 keV.

DISCLAIMER

Table 1. Plane Polarized Soft X-ray Undulator Parameters

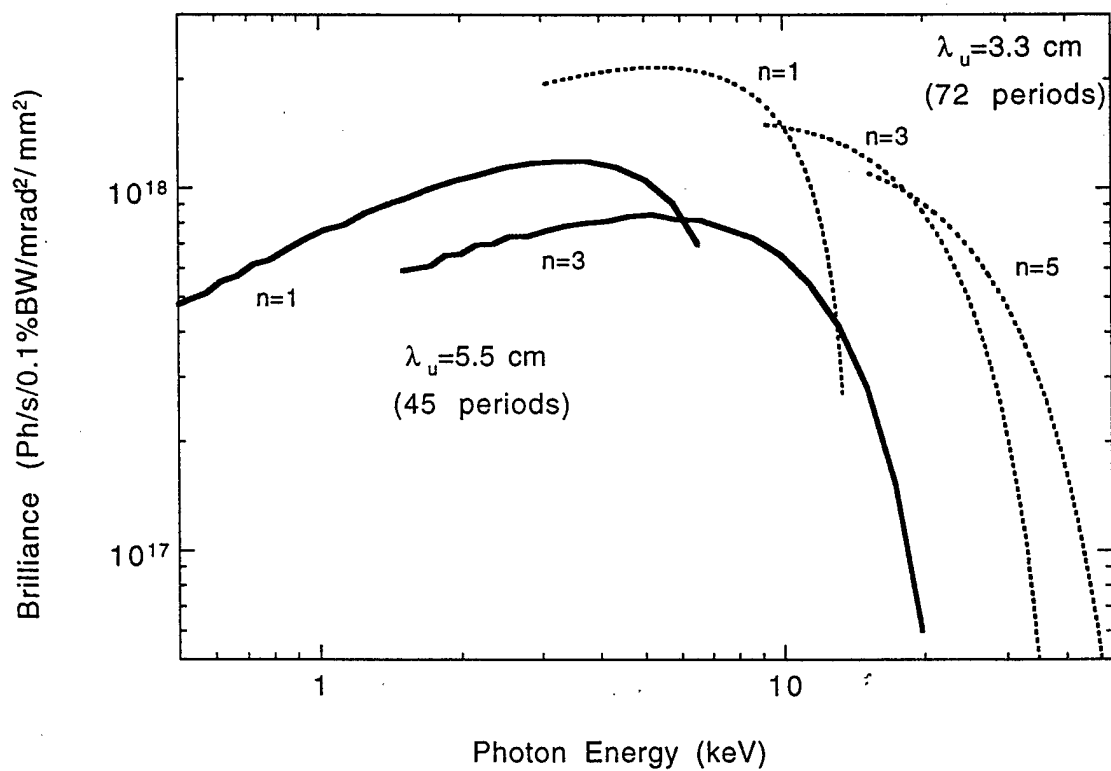| Length	2.4	m
Period, λu	5.5	cm
Minimum gap	11.5	mm
Maximum Deflection Parameter	5.7	
First Harmonic Tuning Range	0.5 - 7	keV
Horizontal Positron Beam Size (σ_x)	346	μm
Vertical Positron Beam Size (σ_y)	45	μm
Horizontal Positron Beam Divergence ($\sigma_{x'}$)	20	μrad
Vertical Positron Beam Divergence ($\sigma_{y'}$)	4.5	μrad

Figure 1. Total flux (upper curve) of the APS 5.5-cm-period undulator and undulator A, calculated for a storage ring energy of 7 GeV and a current of 100 mA. The 5.5 cm device has 44 periods, the gap is set at 11.5 mm (K=5.67) to give a first harmonic peak at 500 eV.

An illustration of the major optical elements relevant to the spectroscopy beamline, 2ID-C, is given in figure 2. A fixed aperture (FA), acting as a pinhole, with dimensions of 4.5 mm x 4.5 mm is located directly downstream of the shield wall. A plane silicon mirror, M1, at 28 m from the center of the 5.5-cm-period undulator, intercepts the beam with a grazing incidence angle of 0.15°. This mirror deflects the beam 0.3° inboard and is shared by all three beamlines. Mirror M2C, at 29.5 m, is the horizontally focusing mirror of the SGM and is used to image the source at the experimental station. The grazing incidence angle is 1.25°, and a rhodium stripe will be used for the energy range up to 2.6 keV. Because of the limited lateral floor space, a smaller grazing incidence angle could not be used. A multilayer will extend the energy range of this mirror to 3 keV. From measurements we have made at NSLS X8A,[7] the nickel-carbon multilayer will cover the 2.6-to-3 keV energy range with a reflectivity of more than 60%. The third optical component in the spectroscopy beamline is mirror M3C, at 39.15 m, with a grazing incidence angle of 1°. This is the SGM vertically focusing mirror, which has a rhodium coating in addition to the bare silicon substrate. The vertical focusing mirror images the undulator source onto the entrance slit, located at 43.5 m. The entrance slit is continuously variable from 5 to 500 μm. The grating chamber contains three spherical gratings, one of which is selected by a precision linear translation mechanism that intercepts the beam at 47.5 m. The first-order diffracted beam is accepted at an included angle of 176° and focused onto the exit slit, which translates to track the focal position as the energy is scanned. The exit slit, which is identical to the entrance slit, is at 8 m from the grating and has a travel range of 800 mm in the beam direction. The first experimental station is located at 58 m. A refocusing mirror and second experimental station, which are not shown in this figure, will be added at a later date.
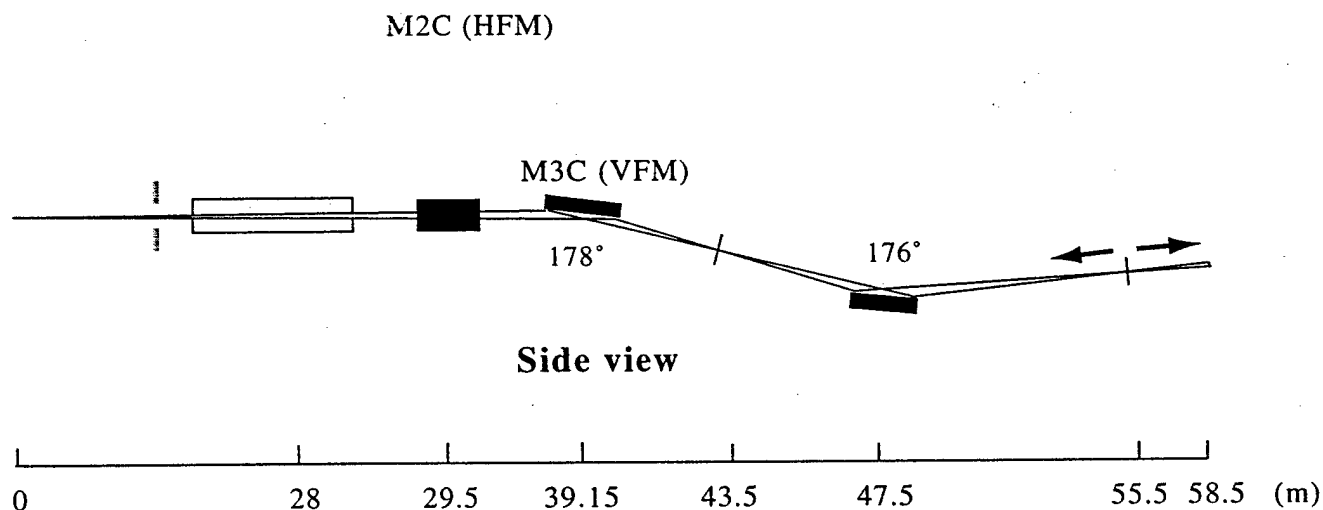

Figure 2. Layout of the APS soft x-ray spectroscopy beamline 2ID-C. The fixed aperture (FA) and M1 plane mirror are primarily used as power filters. Mirrors M2 and M3 are the SGM horizontally and vertically focusing mirrors, HFM and VFM, respectively. The positions of the entrance slit, grating, translatable exit slit, and experiment are also shown.

3. HIGH HEAT LOAD INSTRUMENTATION

Operation of a soft x-ray undulator on a high-energy storage ring, such as the APS, has one potentially limiting factor, namely extremely high total power output. Soft x-ray programs at the ESRF and SPring-8 have circumvented this problem from the beginning by using circularly polarized undulators, with inherently low high harmonic production. At the APS, the maximum power output of the 2.4-meter-long, 5.5-cm-period planar device will be 12 kW. For the APS SXR circularly polarized undulator, this will decrease to approximately 800 W, with identical brilliance in the first harmonic.

Although the total power output of the plane-polarized device presents a formidable problem, we have made significant instrumentation advances. First, a fixed aperture is used to reduce the on-axis power to less than 1500 Watts, and second, a plane mirror reduces the power on the critical monochromator components to less than 400 Watts.[8] Advanced high heat load instrumentation developed for 2ID-C include:

1) A high efficiency "pin-post" cooled silicon mirror,[9] which is expected to achieve a total slope error of less than two microradians with an absorbed power of 2 kW and power density of 350 W/cm^2;

2) Water-cooled entrance and exit slits have been developed as a joint collaboration between the APS and the Advanced Light Source[10] featuring a state-of-the-art Glidcop monolith that is 1.5" thick and 8" in diameter, and has been electric discharge machined to form a complex flex-hinge structure that produces an extremely precise parallel slit motion. Simultaneously this structure acts as a high thermal conductivity path, removing power from the slit to integral water-cooling channels;

3) The monochromator, manufactured by Physical Science Laboratories, with water-cooled gratings is similar to that installed on the ESRF soft x-ray spectroscopy beamline.[11]

4) In collaboration with Peter Takacs (BNL) and Werner Jark (Trieste), we are developing an *in-situ* long trace profiler that will measure mirror surface profiles in a UHV environment while the mirror is subjected to high power x-ray beams.[12]

4. HIGH RESOLUTION MIRROR ACTUATION SYSTEM

In addition to the high heat load requirements of the beamline optical elements, we also have to consider additional conditions, such as high stability, resolution and repeatabilty, necessary at a third-generation source. The most severe requirements for the 2ID-C SGM are at the vertical focusing mirror. In the present geometry, with a 9:1 vertical demagnifcation onto the entrance slit, we expect to acheive a source image of approximately 30 µm, including aberrations. For high-resolution operation of the monochromator, the entrance slit will be set to approximately 5 µm. Intensity fluctuations due to beam movement at the slit must be minimized. This means that the mirror must have high thermal and vibration stability. At the same time, to maximize the transmitted intensity, the image must be stepped with sufficient resolution. In the present design, we considered that, with a mirror-to-slit seperation of 4.35 m, we required a mirror pitch resolution of < 25 nrad. Since no commercially available actuation system was available, we decided to build our own system. The concept, which we call a "virtual sine arm system", is undergoing patent application and is presented seperately in these proceedings.[13] With this system, we have inferred, from interpolation of measurements, that we have a single step resolution of < 0.4 nrad.

5. CALCULATED RESOLUTION, FLUX AND HARMONIC SUPPRESSION

By optimizing the demagnification ratio to balance the requirements of: 1) high transmission through the entrance slit, 2) maximum resolving power, and 3) minimum exit slit travel range, we have chosen to use a 9:1 vertical demagnification ratio. Given this optical geometry, the predicted total resolving power of the SGM is shown in figure 3 for three gratings of 600, 1200, and 1800 lines/mm. In this calculation, the grating slope error is assumed to be 1 µrad RMS, and the entrance and exit slits are both 5 µm. The exit-slit translation, along the beam direction, is less than 800 mm in all cases.

Assuming a conservative grating efficiency of 5% and taking into account the first harmonic intensity, pinhole transmission, mirror reflectivity, and slit throughput, the intensity at the experimental end station will be approximately 10^{13} photons/s/0.1%BW with a beam size of 1 mm^2. At a resolving power of 5000, we expect an intensity of more than 10^{12} photons/s.

For many spectroscopic applications, it is very important to have a pure first-order monochromatized x-ray beam. Because the SGM, unlike a plane-grating monochromator, has no degree of freedom to eliminate high diffraction orders, we plan to reduce the harmonic content from the source by using the cutoff energies of the mirror coating materials.[14] Reducing the intensity of high harmonics prior to monochromatization will reduce the intensity of high orders at the sample. Calculated suppression of second and higher orders is approximately a factor of 30 to 400 smaller, relative to the first harmonic.
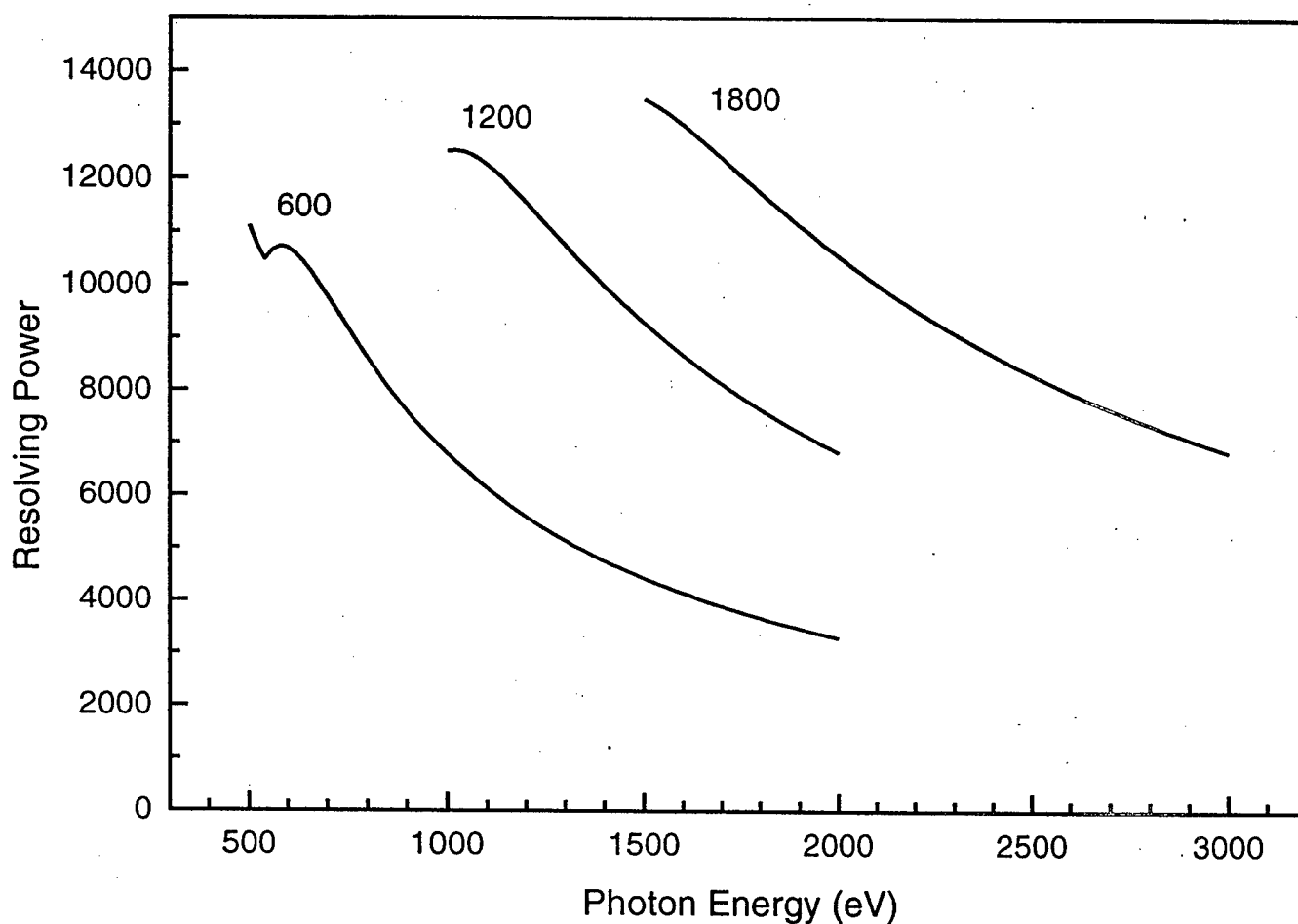

Figure 3. SGM resolving power with 9:1 demagnification, 10 mm slits, and gratings of 600, 1200, 1800 lines/mm, each with a slope error of 1 mrad. The curves are calculated only for an exit slit travel range less than 800 mm.

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