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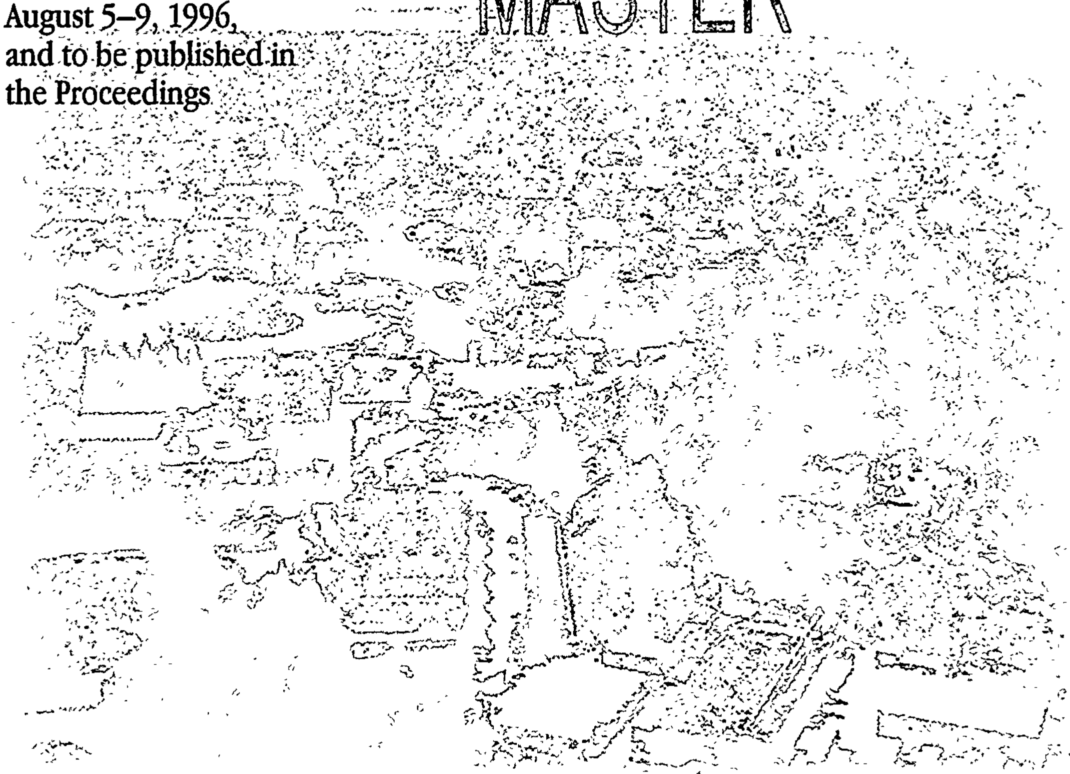

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ELLIPTICALLY POLARIZING UNDULATOR BEAMLINE 4.0.1 FOR MAGNETIC SPECTROSCOPY AT THE ADVANCED LIGHT SOURCE*

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DISCLAIMER

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ABSTRACT

A beamline for high resolution spectroscopy with elliptically polarized X-rays is described. The working energy range is large, from 20 eV to above 1800 eV. The resolving power is on the order of 10,000 at low energies (20 eV– 200 eV) and 6000 at high energies (200 eV–1800 eV). This is achieved using a variable deviation angle plane grating monochromator. A single grating, with one line density and a varying groove depth, is used to cover the entire energy range. The beamline has been designed to operate with either one or two x-ray beams propagating simultaneously through the monochromator and to the experimental station. Switching between polarizations at rates of 0.1 Hz and slower is accomplished in the single beam mode by alternating the output of the elliptically polarized undulator source between left and right polarization. Fast polarization switching, at rates of 100–1000 Hz, is provided in the two beam mode by mechanical chopping between two photon beams, one of which is right circularly polarized, and the other left circularly polarized.

Keywords: soft X-rays, monochromators, elliptically polarizing undulators.

1. INTRODUCTION

The application of circularly polarized x-rays to studies of chemistry and physics has recently become a field of intense interest. Circular dichroism experiments use the differential absorption of left versus right circularly (or elliptically) polarized x rays to probe the structure, physics, and chemistry of a variety of materials. Studies of systems as diverse as magnetic materials, biological molecules, and monolayer/thin film structures have been performed using circularly polarized x-rays. From these studies, information such as the magnetic moment and the structural environment of the system can be measured. Circularly polarized x-rays have also been used to image magnetic structures. Magnetic microscopy has been used to create element specific images of the magnetic domains of interest to the semiconductor/magnetic recording industry.

The Advanced Light Source at Lawrence Berkeley National Laboratory is designing and building a complement of insertion devices and beamlines to facilitate this research. Using undulators which directly produce circularly polarized light, high flux, high brightness beams of x-rays will be available at "application-specific" beamlines. Up to four undulators will be used to produce the radiation for two independent beamlines, one for high resolution spectroscopy and one for microscopy. This approach allows the optical designs to be optimized for the differing requirements of these two applications.

In this paper the design of one of these two branches, the magnetic spectroscopy branchline, Beamline 4.0.1, is described. First, the experimental requirements and design features are presented. Second, the considerations leading to the monochromator design are given. Finally, the design of the beamline as a whole is presented.

2. EXPERIMENTAL REQUIREMENTS

The beamline design has been optimized for spectroscopy experiments over a wide energy range. The design energy range is 20 eV to 1800 eV, with a resolving power of 10,000 at 20 eV and 6000 at 1800 eV. The large range is required for conducting valence band mapping studies at low energy and high resolution core level spectroscopy at high energy. An essential feature is that tuning the energy over the whole energy range must be accomplished rapidly, with a minimum of grating changes and without recalibration. Circular dichroism experiments measure the difference in absorption between left and right circularly polarized light and, in generally, require that two separate spectra be obtained, one with left and the other with right polarization. The two spectra are then subtracted from each other to produce the dichroism spectrum. This subtraction makes these experiments sensitive to small variations in the photon energy, intensity, and polarization, and leads to the requirement that the stability and reproducibility of the monochromator be very high.

A novel feature of this beamline is that it is possible to have separate x-ray beams from two independent undulators propagating through the beamline simultaneously and coming together at the sample. A pair of elliptically polarizing undulators are the sources of x-rays for this beamline. These insertion devices directly produce elliptically polarized radiation of any desired helicity. By adjusting the longitudinal position of the magnet rows in the undulator, the polarization of light can be varied from horizontal or vertical linear to left or right circular polarization. However, even though this switching is automated and under user-control, the adjustment takes a finite time (a few seconds,) so that the rate of polarization switching using one undulator is limited. For experiments which require faster switching, two undulators can be used in this beamline, with one undulator adjusted for one polarization and the other adjusted for the opposite polarization. With both beams going through the beamline simultaneously, switching can be accomplished by mechanically chopping the beams, alternating between the two polarizations. This can take place at rates of a thousand hertz or more, but for best results, the technique requires that both beams be as close as possible in energy, degree of polarization, and size. Satisfying this requirement is challenging and adds to the beamline complexity.

Finally, in addition to the energy range and resolution requirements, different types of experiments utilize different beam sizes at the sample. For example, angle resolved photoemission studies benefit from a tightly focused beam which matches the small field of view of most electron spectrometers, while fluorescence spectroscopy of metalloproteins requires a defocused beam to minimize radiation damage. This leads to the use of adaptive refocus optics. By using a mirror which can vary its focal length, the size of the x ray spot at the sample position can be changed.

3. MONOCHROMATOR DESIGN

Several alternative types of monochromators were studied, principally the spherical grating monochromator (SGM) [1], the variable angle SGM, [2] and the variable angle plane grating monochromator (PGM) of Petersen.[3] An SGM has only one optical element, a grating, with the great potential for increased efficiency. However, the energy range of a single grating is limited, and to cover the desired energy range at high resolution would require a large number of gratings. Although the variable angle SGM has the advantages of an extended energy range and of fixed slits in comparison to the normal fixed included angle SGM, this design would still require the use of three or more gratings. The only solution which can cover the very large energy range with the desired spectral resolving power and a minimum number of gratings is the variable angle PGM, such as the SX-700. Traditionally, this monochromator design uses two gratings to cover the energy range required for this beamline, one with relatively low line density for the low photon energy range, and one with higher line density for the higher photon energies. The primary disadvantage of this design compared to the SGM is the additional two reflections needed, one from the pre-mirror needed to vary the included angle, and the second from the focusing (spherical or elliptical) mirror which focuses the diverging light from the grating onto the exit slit.

Even this design can be improved, though. Diffraction efficiency calculations [4,5] show that one grating can cover the entire energy range if the groove depth can be varied. In fig. 1 the diffraction efficiency of a 700 l/mm grating with a varying groove depth is shown. The solid line shows the efficiency obtainable if the groove depth continuously changes from 60Å to 600Å. This curve is obtained by reoptimizing the groove depth for each energy. To practically apply the variable groove depth concept, the grating could be manufactured with the groove depth varying across the width of the grating. The desired groove depth would be selected by translating the grating sideways so that the photon beam illuminates only the "strip" of grating which has the required depth. If the groove depth continuously varies across the width of the grating, the optimum depth for any given energy could always be selected, giving the highest efficiency. However, this concept has the disadvantage that different portions of the photon beam, which is of finite width, would illuminate a range of groove depths, leading to one portion of the beam being diffracted less efficiently than another. For this reason, a grating which is stepwise variable across its width has been specified. A grating with seven grades in groove depth has been chosen. Fig. 1 shows the diffraction efficiencies for this grating. The efficiency is about 15-20% over the entire energy range. This approach is possible as we are using a highly

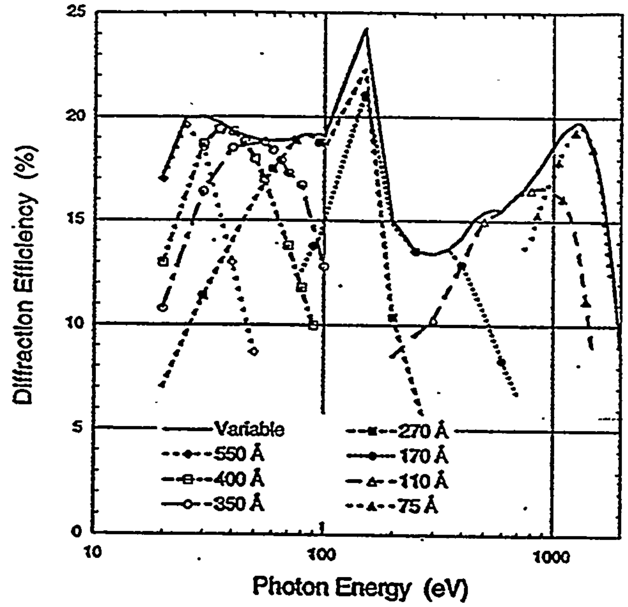


Figure 1 Diffraction efficiency of the grating with variable groove depth. The solid line is for a continuously variable depth, while the other lines are for discrete values as noted. The grating has a line density of 700 l/mm, a groove width of 10000 Å, and is gold coated.

collimated undulator source, with a beam width at the grating which is much smaller than the nominally specified grating width.

To produce a grating with a variable groove depth, almost all of the existing processes of fabricating a conventional holographic grating can be used. This includes the photoresist chemistry, the necessary interferometry, and the etching technology. In order to vary the groove depth, only the etching time needs to be adjusted. By etching portions of the grating for a longer time, the grooves are made deeper. One method that can accomplish this to use a shutter to selectively mask portions of the grating, so that different portions of the grating are exposed to the etching plasma for different times. Several grating manufacturers have made or have techniques to make such gratings.

The choice of line density is made on the basis of the source size, the allowed pre-optics demagnification, and the length allowed from the entrance slit to the grating. The source size, in the case of this beamline, includes a contribution by diffraction, as the electron beam is smaller than the diffraction limited size at the lower photon energies reached by this beamline. This source-size limited resolving power is the resolution obtainable with the monochromator slit widths set equal to the size of the photon beam, giving the highest efficiency for the design resolution. The apparent source size is also determined by the monochromator demagnification, which in turn is limited by the allowed size of the rest of the optics and the scaling of the monochromator aberrations with the vertical aperture. Finally, the slit-to-grating distance is dependent on the total space available for the entire beamline. For this beamline, the design constraints have led to the selection of a grating with a groove density of 700 l/mm. Figure 2 shows the included angle and the grazing incidence angle for the monochromator. Figure 3 shows the calculated resolving power of the monochromator with this grating under three limiting conditions: a) resolution limited only by source-size; b) resolution set by the coma of the grating; and c) resolution limited by the coma aberrations of the spherical mirror. The methodology used for calculating these terms is given elsewhere.[6] As can be seen, the resolving power is limited by different effects depending on the energy. At lower energies, the resolution is set by the coma aberrations of the grating, which limits the resolving power to approximately 10,000. At higher energies, the aberrations become less significant as the divergence of the undulator source decreases. At these energies, the resolution is given by the source-size limited value of approximately 6000. (It should be noted that the source-size limited resolution is calculated assuming the monochromator slits are set to the full width half maximum points of the demagnified source. However, in practice, the slits will generally be closed to smaller widths giving not only a reduction in the amplitude fluctuations caused by source motion, but also yielding a higher resolving power.)

For the variable angle PGM, the virtual source-to-grating distance r' is given by $r'=r \cdot K^2$, where r is the actual slit-to-grating distance and $K=\cos\beta/\cos\alpha$, a constant. By fixing K, the exit slit is fixed and high resolution is obtainable over a wide energy range. K is generally selected to maximize the diffraction efficiency over the energy range desired. For the monochromator discussed here, K=2.24, which gives an entrance arm 5 times the actual source distance. The monochromator under design has been specified to have an entrance slit to reduce any problems caused by source motion, so that the real source-to-grating distance is 4 meters, and the virtual source is at 20 meters. To avoid the use of an elliptical focusing mirror (which would have larger slope errors than a spherical mirror and thus cause a resolution decrease,) the exit arm for the monochromator is set at 9 meters, giving a demagnification of 2.5 by the spherical focusing mirror.

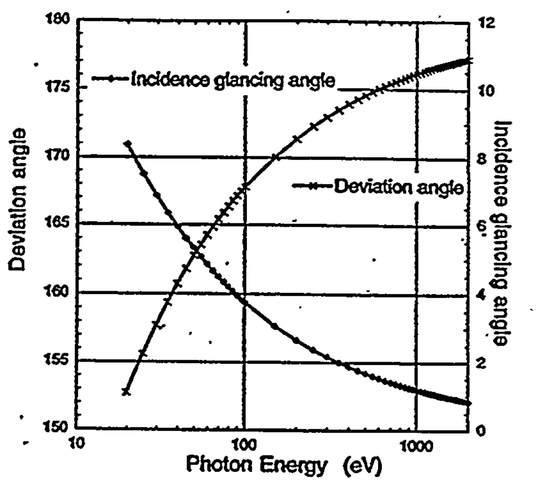


Fig. 2. Included and glancing incident angles versus the energy.

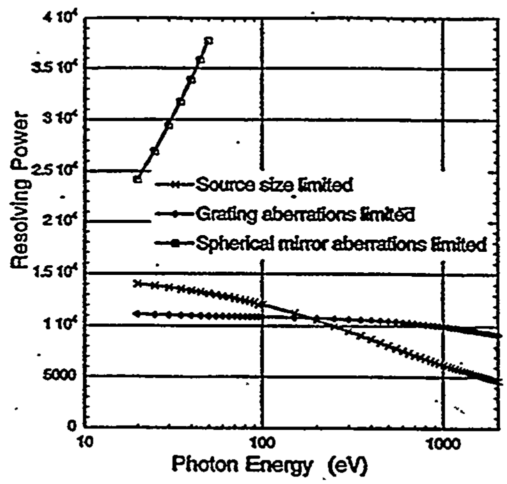


Fig. 3. Resolving power limited by the source size and aberrations of the grating and refocusing spherical mirror.

Ray tracing of the PGM design using positive order was carried out with the program SHADOW.[7] Fig. 4 shows the results at a number of energies. The monochromator parameters are r=4 meters (i.e. the entrance slit-to-grating distance), N=700 l/mm, m=+1, and K=2.24. A gaussian distribution for the source spatial and angular distributions has been used, in good approximation to an undulator source. For each nominal energy E two additional energies of ±ΔE were also traced. ΔE corresponds the calculated resolving powers shown in figure 3. As can be seen , in all cases the lines are well resolved, confirming the high resolution capability of the design. The image at the exit slit for three energies for particular resolving power at every energy is shown in the figure.

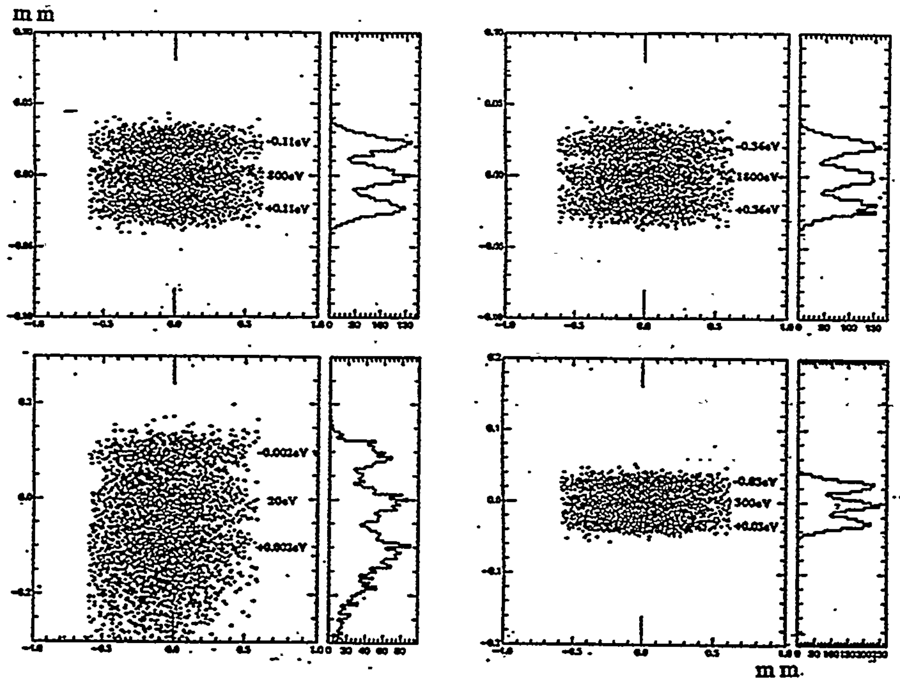


Figure 4 Ray tracing results for the image of the source on the exit slit at different energies. The energy offsets are calculated from the predicted resolving power as shown on figure 3.

A final design option being studied is the use of a variable line space [8-10] (VLS) grating. With this type of grating, the virtual source distance r' produced by the grating is approximately constant for all combinations of α and β, not just for a constant K. This would allow the grating angles to be optimized for other than focus considerations, such as for diffraction efficiency or higher order suppression. The recent advent of high quality holographic VLS gratings has made the use of these gratings a viable option for x-ray applications. Studies of the performance of these gratings in this beamline are currently being performed.

4. BEAMLINE DESIGN

After selection of the monochromator, the biggest challenge in designing the beamline is the requirement for fast chopping between left and right polarization. As discussed earlier, polarization switching which occurs faster than 0.1 Hz will be accomplished by propagating two separate beams down the beamline, one set for one helicity and the other of opposite helicity. Polarization switching is then rapidly changed

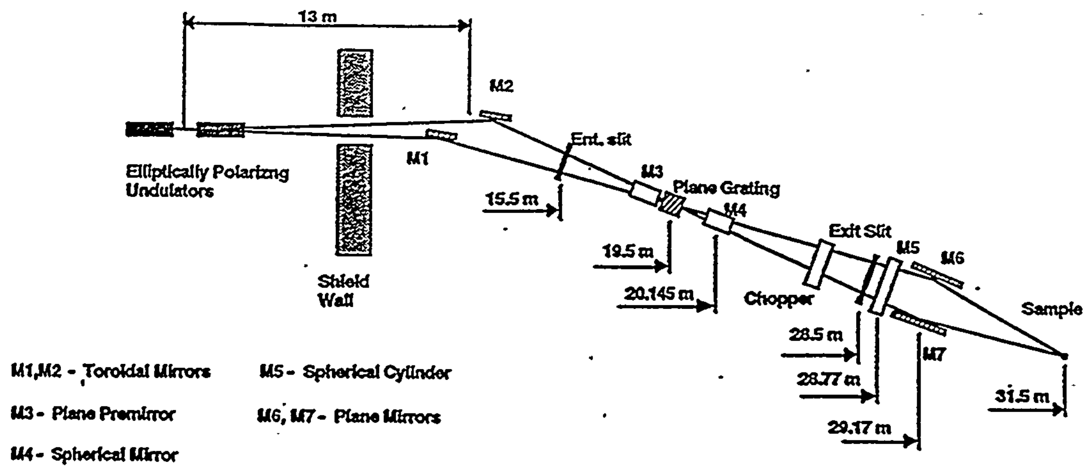
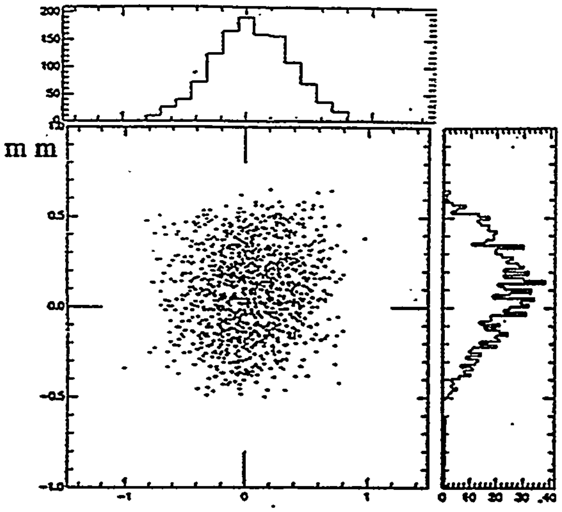


Figure 5 Schematic layout of Beamline 4.0.1

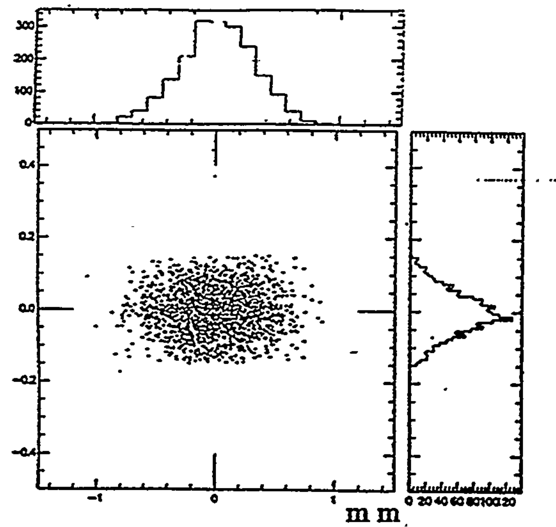
by using a chopper to alternate between the two beams. These beams must have the same energy, degree of polarization, and shape and hit the sample at the same spot. By having the beams go down the same beamline and sharing as many optical components as possible, this requirement is more easily met.

The layout of the beamline is shown in figure 5. The elliptically polarizing undulators[11,12] are located in a single insertion device straight, where two "undulator stations" are placed end-to-end. Small bending magnets produce a "chicane" in the straight section, giving a 2.5 mrad angle between the two optical axes. Undulators can be operated at both stations simultaneously. In addition, at each station, a translation mechanism will allow either of two undulators to be placed in the beam. The output from either undulator station can be directed to either branch line, or the output from both stations can be set down the same branch line simultaneously.

The two beams with right and left polarization from the undulator sources are focused by two toroidal mirrors onto the entrance slit. The toroidal mirrors focus sagittally in vertical direction onto the entrance slit and tangentially in the horizontal direction onto the sample. The advantage of having a toroidal mirror instead of a more traditional Kirkpatrick-Baez configuration is that there is only one reflection instead of two. The small divergence from the undulators allows the use of sagittal focusing with only small



(a)



(b)

Figure 6 The image of the beam at the sample position for: a) 20 eV, b) 800 eV

aberrations. It should be noted, though, that this configuration requires the yaw angle and vertical position be very stable, on the order of 20μrad and 2μm, respectively. Errors of these magnitudes cause the demagnified image of the beam on the entrance slit to rotate or translate on the order of 10% at high energies.

As discussed above, the monochromator is a variable angle PGM. The included angle is varied by translating and rotating a premirror. At the same time, the grating is rotated to maintain the constant focus condition $K = \cos(\beta)/\cos(\alpha)$. The grating produces a "virtual entrance slit" at a distance equal to $r' = r \times K^2$, where r is the real entrance slit-to-grating distance and α and β are the incidence and diffraction angles respectively. In our case r = 4m and K = 2.24, so r' = 20.07m. The spherical mirror at 0.6m from the grating focuses the virtual entrance slit onto the exit slit. Keeping K constant fixes the position of the virtual entrance slit, which also fixes the position of the exit slit. The large virtual source position precludes the use of 1:1 focusing for the spherical mirror, and so some coma results. However, as shown in fig. 3, the major contribution to coma aberrations comes from the grating rather than the focus mirror.

Emerging from the exit slit, the photon beams are vertically small (tens of µm's) and divergent, while horizontally large (about 1 mm) and convergent. Although the horizontal size is appropriate for spectroscopy applications, the vertical size is, in general, too small. The beams are therefore vertically refocused using a cylindrical mirror and horizontally deflected using plane mirrors to the sample. The cylindrical mirror is placed to give beam *magnification*, so that the vertical size is on the order of 0.5 mm. Because this mirror is located close to the exit slit, the size of the beam incident on the mirror is small, allowing the use of a 1° grazing angle of incidence. The two plane mirrors steer the two beams horizontally to the same spot at the sample. The grazing angle on these mirrors is also very small, about 0.7°. Because of these shallow incidence angles, the net reflectance for the two reflections is high, with a larger value than a single optic with 2° grazing angle.

Fig. 6 shows the beam spots at the sample position for 20 eV and 1800 eV. One can see that at low energies the beam size is equal to $\approx 1 \times 1$ mm^2, vertical x horizontal, while at high energies it is equal to $\approx 0.2 \times 1$ mm^2. This variation in vertical size is due to the fact that the vertical beam size is diffraction-limited, and hence energy dependent, at some energies. This variation, although not a critical fault, makes it difficult to match the beamsize to the experiment if a large range of energies is required. In addition, the wide variety of experiments scheduled to use this beamline have differing vertical size requirements. For this reason, we are planning on making the cylindrical mirror a bendable mirror. With this optic, the focal distance of the mirror can be adjusted.[13] Experimenters who desire a small beamsize can adjust radius to place the focal point at the sample position, while researchers who desire larger beams can defocus the mirror to produce a larger spot.

5. CONCLUSION

The design of beamline 4.0.1 for high resolution magnetic spectroscopy at the ALS is described. A variable angle plane grating monochromator (PGM) has been adopted. By using a novel grating design which has a variable groove depth, high diffraction efficiency of 15-20% can be obtained throughout the wide energy range using only a single grating. Ray tracing has shown that the resolving power is about 10,000 at lower energies (20 eV to 200 eV) and about 5000-7000 at higher energies (200 eV to 1800 eV) with a grating of 700 l/mm. Application of a variable line space grating in this beamline is also being studied.

The beamline uses elliptically polarizing undulators as the radiation sources. These undulators directly produce circularly polarized radiation with high brightness. The beamline design allows for the use of two of these insertion devices simultaneously, delivering two beams with identical energy but opposite polarization properties to the same spot at the sample. With this design, a mechanical chopper can be used to alternately block one beam or the other, producing fast polarization switching at the sample. Table I describes the optics to be used in this beamline. It is scheduled to begin operatation in 1997.

6. ACKNOWLEDGMENTS.

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Table I

	Component	Description	
M401.1	Horizontally deflecting mirror from the first undulator Focuses beam to the entrance slit vertically and to the sample horizontally	Water-cooled Toroid Sagittal radius Longitudinal radius Footprint Glancing angle	 150.5 mm 471.557 m 140x5 mm 1.911425°
M401.2	Horizontally deflecting mirror from the second undulator Focuses beam to the entrance slit vertically and to the sample horizontally	Water-cooled Toroid Sagittal radius Longitudinal radius Footprint Glancing angle	 141 mm 403.518 m 140x5 mm 2.08312°
	Monochromator	Variable angle PGM	
S401.1	Entrance slit.	Water cooled Footprint	 22 mm
M401.3	Plane premirror	Water cooled Deviation angle	 153°–177°
G401	20 eV—1800 eV Deviation angle Grating	Au, 700 l/mm Groove width Groove depth Footprint	 1000 nm 5-60 nm 80x4 mm
M401.4	Vertically focusing postmirror Focuses on the exit slit	Spherical Radius Footprint Glancing angle	 342.584 m 400x4 mm 2°
S401.2	Exit slit	Footprint	40 mm
M401.5	Vertically focusing mirror. Focuses the beam on the sample.	Spherical cylinder Radius Footprint Glancing angle	 28.157 m 40x40 mm 1°
M401.6	Horizontally deflecting mirror. Steers the beam onto the sample.	Plane Footprint Glancing angle	 200x1 mm 0.6778°
M401.7	Horizontally deflecting mirror. Steers the beam onto the sample.	Plane Footprint Glancing angle	 200x1 mm 0.6591°