Beam Collimation using Polycapillary X-ray optics for Large Area Diffraction Applications
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Abstract
Polycapillary optics, arrays of thin-walled, hollow borosilicate glass channels, can be employed to redirect, collimate and focus x-ray photons. Polycapillary collimating optics collect x-rays over a wide solid angle (as large as 10-15 degrees cone angle) and a large energy bandwidth and provide a quasi-parallel beam with a small divergence (a few milliradians). Parallel beam geometry and uniform local divergence give symmetric uniform peak shapes. This combined with the diffracted beam intensity gain allows accurate analysis of thin complex multilayer diffraction peaks. Experimental results are compared to Monte-Carlo geometrical optics simulations to study performance characterization of polycapillary collimating optics. In-situ thin film growth monitoring times, utilizing x-ray diffraction, could be reduced significantly by employing capillary optics. Suppression of higher energy Bremsstrahlung and background rejection accompanied by the benefit of increased tube potential enhances the signal to noise ratio for thin film analysis.

Introduction
Polycapillary x-ray optics are composed of glass fibers, each made up of hundreds of hollow thin walled channels. Grazing incidence x-ray photons are guided along these microchannels by total reflection, ¹ as exploited in grazing incidence mirrors commonly used on synchrotron beam lines. The reflectivity of these channels remains high as long as the glancing angles are kept below the critical angle for total external reflection, θ_c. ² The channels must be gently curved and kept small enough that the maximum angle of incidence is kept smaller than the critical angle θ_c, as illustrated in figure 1. The reflectivity is higher at smaller angles, even at angles below the critical angle. The critical angle θ_c in mrad, for borosilicate glass is expressed as

\[ \theta_c \approx \frac{32}{E} \]  

where E is the photon energy in keV. The radius of curvature, R, of the polycapillary fiber and the angle of incidence, θ, are related through the equation

\[ \theta \equiv \sqrt{\frac{2d}{R}} \leq \theta_c . \]  

Since the critical angle θ_c is inversely dependent on the photon energy, efficiently transporting high-energy photons requires channels with small diameters, d, and small bending. Figure 2a is a micrograph of a polycapillary fiber cross section. Thousands of these fibers are strung through grids to form a multi-fiber optic as shown figure 2b.

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Transmission

Transmission of an optic is the ratio of the number of photons exiting at the output end of the optic to the number incident at the input. Transmission through a fiber depends upon the fractional open area, the reflectivity for each reflection, and the number of reflections. The fractional open area of a fiber is the part of the input cross-section that is open; not blocked by the glass walls that delineate the channels. Typical open areas of fibers lie between 60 – 75 %. Fig 3a displays a Polaroid image of the output of multi-fiber optic I. Subsequent to this photograph, part of this optic had been subjected to the white beam at the National Synchrotron Light Source (NSLS) at the Brookhaven national laboratory, and a few fibers were removed for radiation damage studies. This part was covered by a 11 X 17 mm² lead rectangle as seen in figure 3b.

The focal distance of an optic is the source-optic distance at which the optic transmission is the highest. The transmission is lower at source optic distances smaller than the focal distance, as only the central straight fibers in the optic transmit and the x-ray photons are incident on the outer fibers at angles larger than the critical angle for total external reflection. Figure 4a displays experimental and simulated transmission as a function of source lens distance for multifiber I. The peak is at 150 mm. The experimental transmission values in figure 4a, for distances less than the focal distance are higher than the simulated results. This may be due to fiber misalignment at the input end of the optic, which results in some fibers pointing to positions farther than the focal point.

The best transmission, at the focal point, as a function of photon energy, is shown in figure 4b. The transmission drops off with energy due to the smaller critical angles at higher energies. The difference between the experimental and simulated curves is due to lens imperfections such as misalignment and waviness.

Waviness ω, is random localized tilting of the channel walls that changes the incident angle at every bounce, thereby affecting the transmission. The waviness parameter ω is the Gaussian width of the normal distribution of tilt angles used in the simulation. The simulations of figure 4 do not include the effects of profile errors such as waviness. Figure 5 shows the transmission at 20 keV of fibers in different positions of the collimating lens simulated using two simulations, with and without waviness. The horizontal coordinate of Figure 5 is the distance of the simulated fiber from the central axis of the lens. Waviness can cause a reduction of about 40 % on the overall transmission efficiency of the collimating optic at 20 keV. Using the simulation model with a waviness of ω = 0.15 mrad, typical for these fibers, and considering all the fractional open areas, the transmission efficiency of the whole lens with the rectangular lead block at 20 keV was calculated as 2.9 % which is much closer to the measured value of 2.7 % than the ideal lens simulated value of 4 %.
Figure 4: (a) Measured transmission (15 – 20 keV) in comparison with simulated transmission values at 15 and 20 keV. The maximum transmission is at the focal point, 150 mm from the source. (b) Experimental transmission efficiencies as a function of energy for multi-fiber collimating optic I with the lead block in place compared to a simulated ideal lens. The measured transmission efficiency of 30% at 8 keV, which was measured before the blockage of the input window using the rectangular lead plate, was scaled down by 7.5%. Waviness and misalignment reduce the measured transmission compared to the ideal lens simulation.

Multi-fiber optic I, with a focal distance of 15 cm, has a linear acceptance angle of 9 degrees, while multi-fiber II, with a focal distance of 100 cm, has an acceptance angle of only 2 degrees. However, multi-fiber optic II transmits significantly higher than multi-fiber I, as shown in figure 6, because the fibers in optic II are less bent. An output image from multi-fiber optic II is shown in figure 3c.

Divergence
The beam exiting the optic is characterized by a divergence that arises from two effects. The first is the local divergence of the x-rays emerging from each channel, usually between $\theta_c$ and $2\theta_c$. There is also fiber misalignment, the deviation of the individual
channel axis direction from the optic axis direction. To measure the divergence, a silicon crystal was rotated to scan the (400) Bragg reflection for Cu Kα radiation. Since the mosaicity and the Darwin width of the silicon diffraction rocking curve are very much smaller than the measured divergence of the x rays, the contribution of the crystal to the rocking curve can be neglected. Fig 7 shows the measured local divergence of the output of multifiber lens I at 8 keV with a 5 mm aperture placed at −15 cm, −10 cm, 0 cm, 10 cm and 15 cm off the axis of the lens. The FWHM of each divergence curve is around 3.9 mrad, which is very close to the critical angle at 8 keV. The systematic peak center shift seen in figure 7 could be caused by the output ends of the fibers being slightly convergent rather than parallel.

Figure 7: Measured local divergence of the output of multi-fiber I at 8 keV.

The widths of the measured divergence curves shown in figure 7 are larger than that predicted by an ideal lens simulation shown in figure 8a. The divergence of the modeled ideal lens is low because the nearly straight central fibers, if perfect, would not increase the divergence above the entrance divergence value due to the source spot size. Figure 8b shows the simulated divergence profile of x-rays exiting from a straight fiber, which has a FWHM of 2.36 mrad. The simulations in figures 4a and 4b did not include the effects of profile defects and waviness. Waviness will increase the angle of reflection for x-ray photons for most bounces inside the channel. Consequently the divergence from the lens increases. Fig 8c shows a simulated transmission of a straight fiber as a function of exiting angle, using a waviness of \( \omega = 0.15 \) mrad.

Figure 8: (a) An ideal whole lens simulation at 8 keV gives a divergence FWHM of 2.5 mrad. (b) For an ideal fiber, the divergence simulation yields a FWHM of 2.4 mrad at 8 keV, and (c) A simulation with a waviness of 0.15 mrad increases the divergence value for an ideal straight fiber from 2.4 mrad to 4.0 mrad.
Waviness of the channels changes the divergence of the x-rays exiting from the center of the lens from about 2.4 mrad to 4.0 mrad.

**Diffraction Gain**

The flux output from a collimating lens is given by

\[ p_{\text{out}} = \frac{T}{4} \tan \left( \frac{\Omega_0}{2} \right) p, \]  

where \( P \) is the source power, \( T \) the transmission, \( r \) the input radius, \( f \) the source to lens distance and \( \Omega_0 \) the capture angle, \( (\Omega_0 = 2 \tan^{-1}(r/f)) \). The simple power gain, compared to a pinhole designed to have an output divergence of \( 2 \theta_c \), is thus,

\[ \text{Output Power Gain} = \frac{T \tan^2 \left( \frac{\Omega_0}{2} \right)}{4 \tan^2 \theta_c} \approx T \left( \frac{\Omega_0}{2 \theta_c} \right)^2. \]  

For a 7° capture angle, 25% transmission, and 8 keV operation, the gain is 66. The potential benefits of collimation were investigated by Kennedy et al. by installing a multi-fiber collimating optic with a 7 degrees capture angle and a 20x20 mm² output in a Philips X-pert MRD diffractometer with a 200 W (20 kV, 10 mA) extended source (0.4X12 mm²), a Cu anode and a 25.4 μm Nickel filter. Figure 9 shows a Ψ scan across a Si <111> diffraction peak with a pinhole and with the multi-fiber optic. Intensity gains of 20x with improved angular resolution were obtained with the capillary optic. The detector employed was smaller than the output beam from the lens. Increasing the detector area from 10x9 mm² to 20x20 mm² would increase the gain to 60, which is in good agreement with the calculated value of 66. An important concern in single crystal thin film growth is the level of strain in the film. Figure 10 shows a comparison between diffraction data taken from a magnetic recording disk, a multilayer thin film, with and without the collimating optic. The thin film peak at 75° is much more symmetric for the with optic case, which allowed accurate peak location, and therefore strain determination.

**Conclusions**

Multi-fiber polycapillary collimating optics collect radiation from a divergent source and redirect it into a quasi-parallel, low divergence beam. The exit angle divergence analysis showed that the output end of one of the lenses was slightly convergent rather than parallel. Simulations indicate the presence of channel waviness and bending and can increase the beam divergence significantly compared to an ideal lens. Diffracted beam signal gains upto two orders of magnitude for thin film samples are obtained with polycapillary optics retrofit into conventional diffraction systems. The parallel beam geometry resulting from polycapillary optic collimation results in peak symmetrization and ease of alignment.
Polycapillary collimating optic
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Crossed slits

34.4 34.4
34.6 34.6 34.6 34.6 35.0 35.0 35.2 35.2

Phi: I
i

40 80 100 (degrees)

Figure 9: Diffraction signal gain on a (100) Silicon wafer. Polycapillary optic (solid line) compared to 1.35 x 1.35 mm² crossed slits (dashed line), from reference 4.

Figure 10: Magnetic recording disk, thin film, 400 Å CoPtCr, 10 μm NiP, Al substrate. The solid line is data taken with the collimating optic whereas the dotted line is the data obtained without an optic, multiplied by 8X to equate the peak heights, and then offset vertically for comparison, from reference 5.

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References