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MONO: A Program to Calculate Synchrotron Beamline Monochromator Throughputs

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Abstract

A set of Fortran programs have been developed to calculate the expected throughput of x-ray monochromators with a filtered synchrotron source and is applicable to bending magnet and wiggler beamlines. These programs calculate the normalized throughput and filtered synchrotron spectrum passed by multiple element, flat un-focussed monochromator crystals of the Bragg or Laue type as a function of incident beam divergence, energy and polarization. The reflected and transmitted beam of each crystal is calculated using the dynamical theory of diffraction. Multiple crystal arrangements in the dispersive and non-dispersive mode are allowed as well as crystal asymmetry and energy or angle offsets. Filters or windows of arbitrary elemental composition may be used to filter the incident synchrotron beam.

This program should be useful to predict the intensities available from many beamline configurations as well as assist in the design of new monochromator and analyzer systems.

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Introduction

A set of programs have been developed to calculate the throughput of monochromating and analyzing elements. The equations used in the calculation are based on Zachariasen's[1] development of the dynamical theory for the Bragg and Laue cases of diffraction for the transmitted (O-beam) and diffracted (H-beam) beams for parallel sided flat crystal plates. Presently, the types of crystals allowed by the program are silicon and germanium. The throughput is the normalized output of the set of crystals as a function of x-ray energy, incident beam divergence in the plane of diffraction, and polarization perpendicular and parallel to the diffraction plane.

This segment of the crystal's dispersion (the relationship of x-ray energy to angle as determined by Bragg's law for the selected reflection) is a section of a Dumond plot[2]. Dumond presented a graphical method for understanding the effects of multiple crystal monochromators arranged in dispersive and non-dispersive geometries.

The throughput is calculated on a linear energy and angle mesh and is not a Monti-Carlo type calculation. The program SHADOW[3], which is a Monte-Carlo ray-tracing program, also has the capability of calculating throughput for x-ray monochromator crystals. However, the crystal type is limited to the symmetric Bragg case.

The default range of energy and angle is based on the mean energy of the monochromator system and the divergence of the incident beam in the diffraction plane (hereafter, referred to as the vertical divergence since the intended application is for synchrotron sources) on the first crystal element. This range includes the intrinsic energy and angle width of the first monochromator element. The default range can be modified by the user.

Currently, up to twenty separate crystal elements are allowed by the program. Each of the monochromator crystals can 1) be a Bragg reflection or Laue transmission type, 2) be asymmetrically cut, 3) be a reflection, H-beam, or a transmission, O-beam, type element, 4) have an angle or energy offset, and 5) have an arbitrary thickness.

The output files created can be used by other programs to graphically display the information or calculate the filtered synchrotron beam through the monochromator system to assess its performance on a specific beamline.

The Program Structure

There are two programs which calculate the throughput of monochromator systems, MONO_T and MONO_B. In function, these programs are identical. The purpose of the MONO_T program is to interactively calculate the throughput with input from a terminal. The MONO_B program receives input from a data file. MONO_T allows the creation of an ASCII disk file which can be edited and used as the input file for the MONO_B program.

Once the throughput has been calculated with either of these programs the photon flux which can be expected through the monochromator can then be calculated by running another program which also has a terminal or input file capability, SYNC_T or SYNC_B. The SYNC programs calculate the synchrotron spectrum in energy, opening angle and polarization which match the parameters in a previously created throughput file. The characteristics of the synchrotron spectrum are set by the storage ring energy, the critical energy of the bending magnet or wiggler source, and the number of magnetic poles of the device. The photon flux is then calculated at each energy, opening angle and polarization component in units of photons per milliampere - horizontal milliradian - electron volt - vertical milliradian. The synchrotron radiation source is based on a single electron in a uniform dipole magnetic field. At this time, no consideration is made for a finite source size. The flux calculated for a multiple pole device is the product of the above dipole flux times the number of poles in the device.

This synchrotron spectrum can then be subsequently filtered by either elemental or composite filters. Input parameters require the thickness and density of each filter material. Composite filters also require that the mass fractions of each element in the composite be known. The attenuation coefficients calculated are based on spline fits to measured data[4] and include photoelectric absorption, coherent and in-

coherent (Compton) scattering cross - sections.

The filtered spectrum is then convoluted with the monochromator throughput to then give the expected photon flux in energy, vertical opening angle and polarization. The SYNC programs are adaptations of an earlier program, PHOTON[5]. All elements (z's of 1 to 100) are allowed as filters or as parts of a composite. An input file for the SYNC_B program can be generated by running the SYNC_T program.

Other programs have been written which display the normalized or synchrotron throughput files produced by the MONO and SYNC programs. One program displays a perspective view of a three dimensional plot. Another program displays a contour plot of the three dimensional data. Both of these programs use the DISSPLA graphics package[6]. This is a proprietary software package and its use requires the computer be licensed. Examples of these programs output are shown in figures 1 through 3. Also, an output file is written which lists all of the parameters which define the monochromating system and includes the total expected synchrotron throughputs when the SYNC program is executed.

Program Examples

Two examples of the programs will be given. The first example is the normalized throughput of a double crystal silicon (111) monochromator operating at an average x-ray energy of 10keV. The vertical beam divergence has been set to 0.1 milliradian. The throughput is shown in figure 1. Figure 1a shows the three dimensional view of the normalized throughput and figure 1b shows the contour plot. Note that the throughput axis is logarithmic. Figure 2 shows the synchrotron throughput of the monochromator system used at the NSLS with a ring energy of 2.5GeV, critical energy of 5.0keV and the spectrum has been filtered by 0.508mm of Be windows. Again the throughput axis is logarithmic for both the three dimensional views.

The next example is that of a four crystal dispersive monochromator system. The first and last pair of crystals are parallel with the second and third crystal set in a dispersive geometry. Again the normalized throughput is calculated for silicon (111) type crystals at 10keV x-ray energy and 0.1 milliradians

of vertical divergence. Figure 3 shows a contour plot of the expected throughput with a logarithmic scale. Note the x-type structure of the throughput which corresponds to the crossing of the dispersion lines of each crystal pair.

Conclusion

These programs should be useful for estimating the performance of existing or planned synchrotron monochromator systems. They have been used to estimate the flux expected from various NSLS beamlines as well as to assess the performance of the transmission filter system reported elsewhere in these proceedings. They have also been used to calculate the flux expected from a high energy Bonse-Hart small angle scattering camera.

The programs should be particularly useful in situations where the estimation of the throughput is difficult. This may include cases where dispersive elements are involved, effects of crystal offsets, asymmetry, large vertical divergence, polarization, and crystal thickness.

A users manual for the programs is currently being written and will be available from the author.

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Figures

Figure 1 Normalized Throughput of a Silicon (111) Double Crystal Monochromator at 10keV X-Ray Energy and 0.1milliradian Beam Divergence.

A) A 3-D Plot of the Normalized Throughput with a Logarithmic Throughput Axis.

B) A Contour Plot with Logarithmic Contour Lines.

Figure 2 Synchrotron Throughput of the Si (111) Monochromator.

The Storage Ring Energy is 2.5GeV with a Source Critical Energy of 5.0keV. The Total Flux Throughput is 9.44×10^8 photons / sec-mA-horizontal mrad.

A) A 3-D Plot of the Perpendicular or Horizontal Polarization Component. Total Perpendicular Flux is 1.28×10^7 photons / sec-mA-horizontal mrad.

B) A 3-D Plot of the Parallel or Vertical Polarization Component. Total Parallel Flux is 9.31×10^8 photons / sec-ma-horizontal mrad.

Both Plots have Logarithmic Throughput Axes.

Figure 3 Normalized Throughput of a Dispersive Four Crystal Monochromator.

All Crystals are Si (111) with an X-Ray Energy of 10keV and 0.1milliradians of Vertical Divergence.

The Two Crystals Pairs are Parallel with the Second Pair set in the Dispersive Mode.

References

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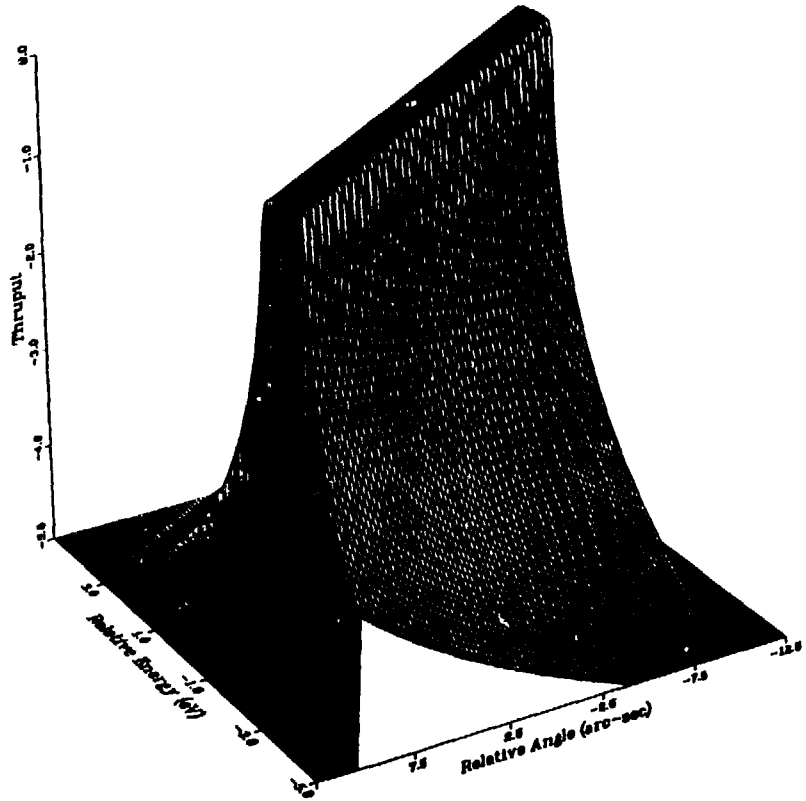
[2] J. W. M. Dumond, "Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power", Phys. Rev 52, (1937) p. 872-883.

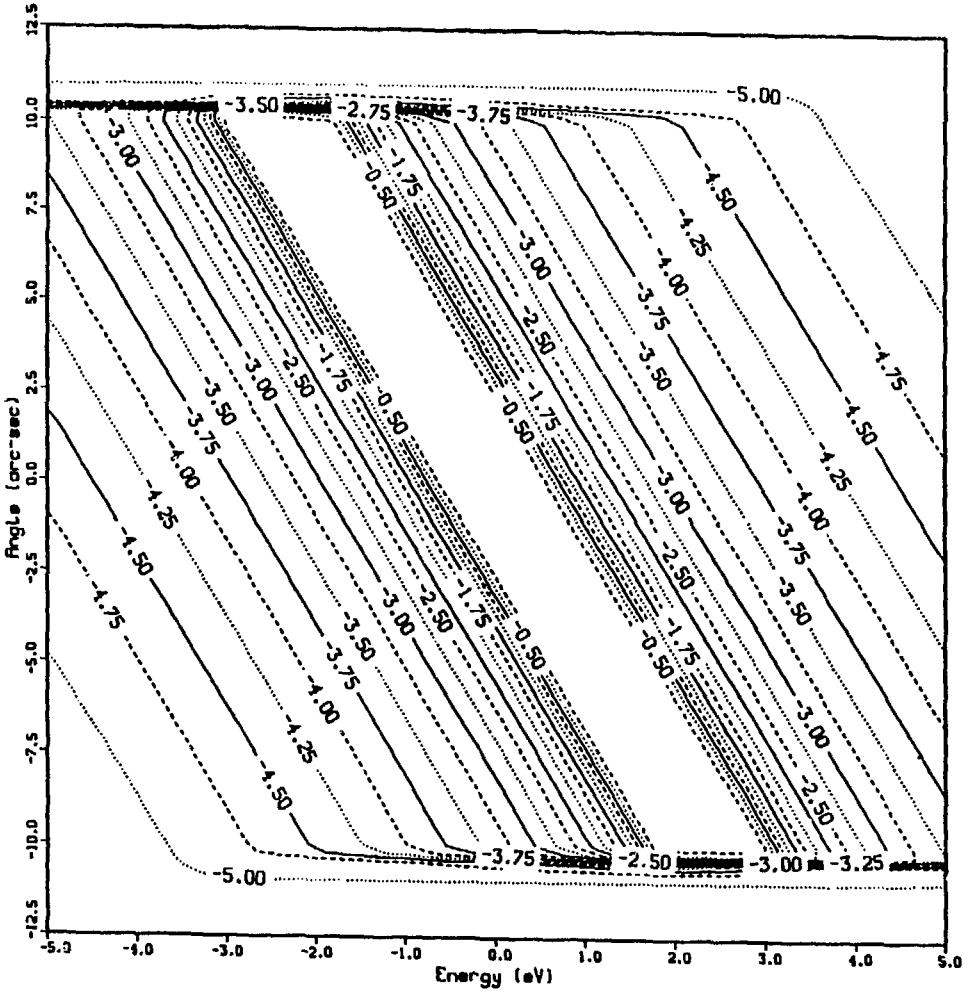
[3] B. Lai, K. Chapman and F. Cerrina, "SHADOW: New Developments", NIM A266, (1988) p. 544-549.

[4] F. Biggs and R. Lighthill, "Analytical Approximations for X-Ray Cross Sections III", Sandia Report, SAND87-0070 UC-34, (1988).

[5] D. Chapman, "PHOTON, A Users Manual", BNL Informal Report, BNL 40822, (1988).

[6] Display Integrated Software System and Plotting Language (DISSPLA). DISSPLA is a proprietary software product of Integrated Software Systems Corporation, San Diego, CA (1977).


Thrupul
Relative Shear (kt)
Relative Angle (arc-sec)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2.5
0.0
-2.5
-5.0
-7.5
-10.0
-12.5
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
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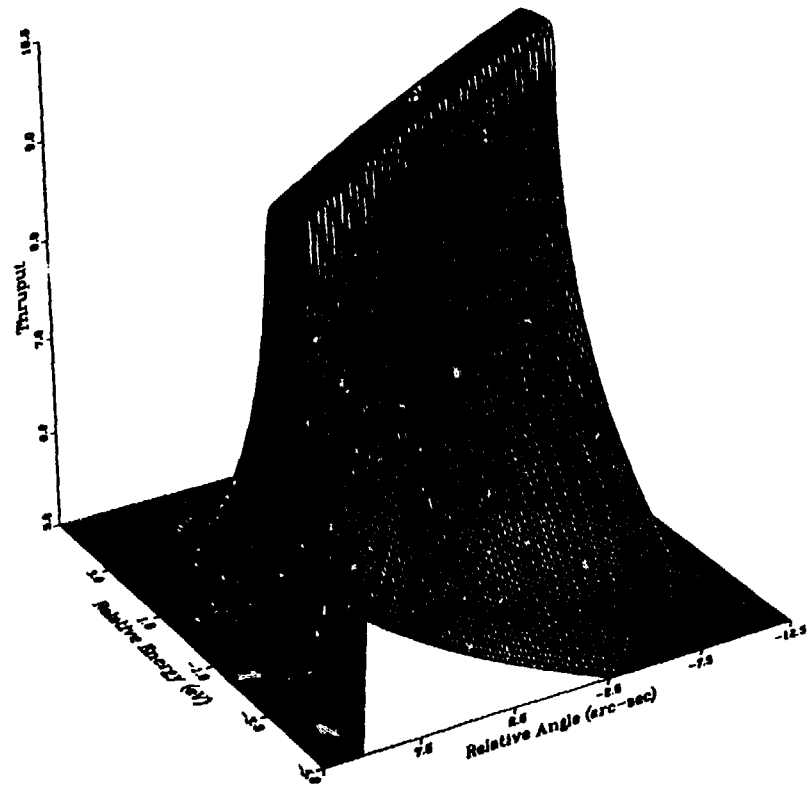
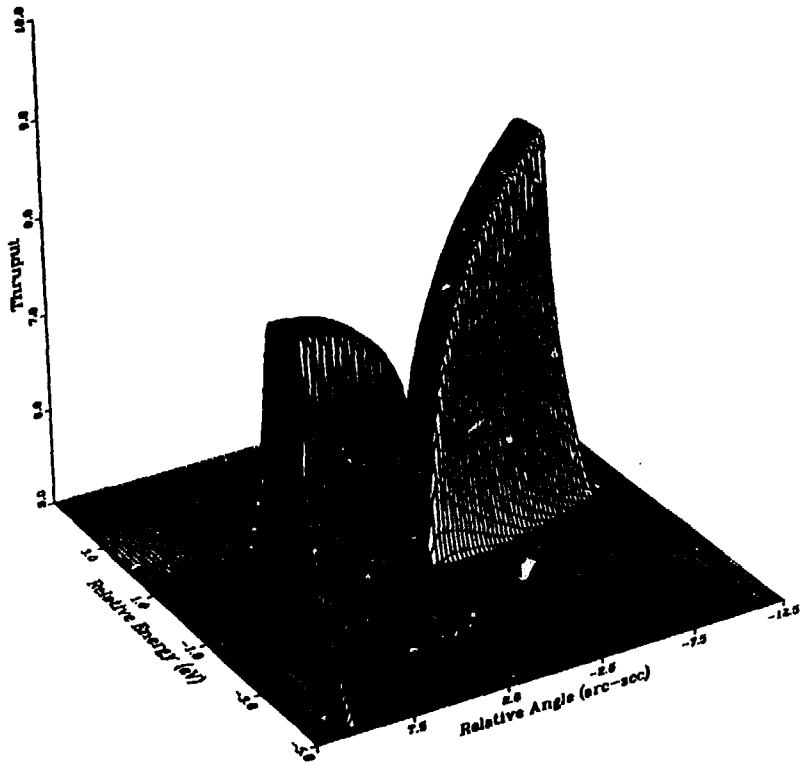
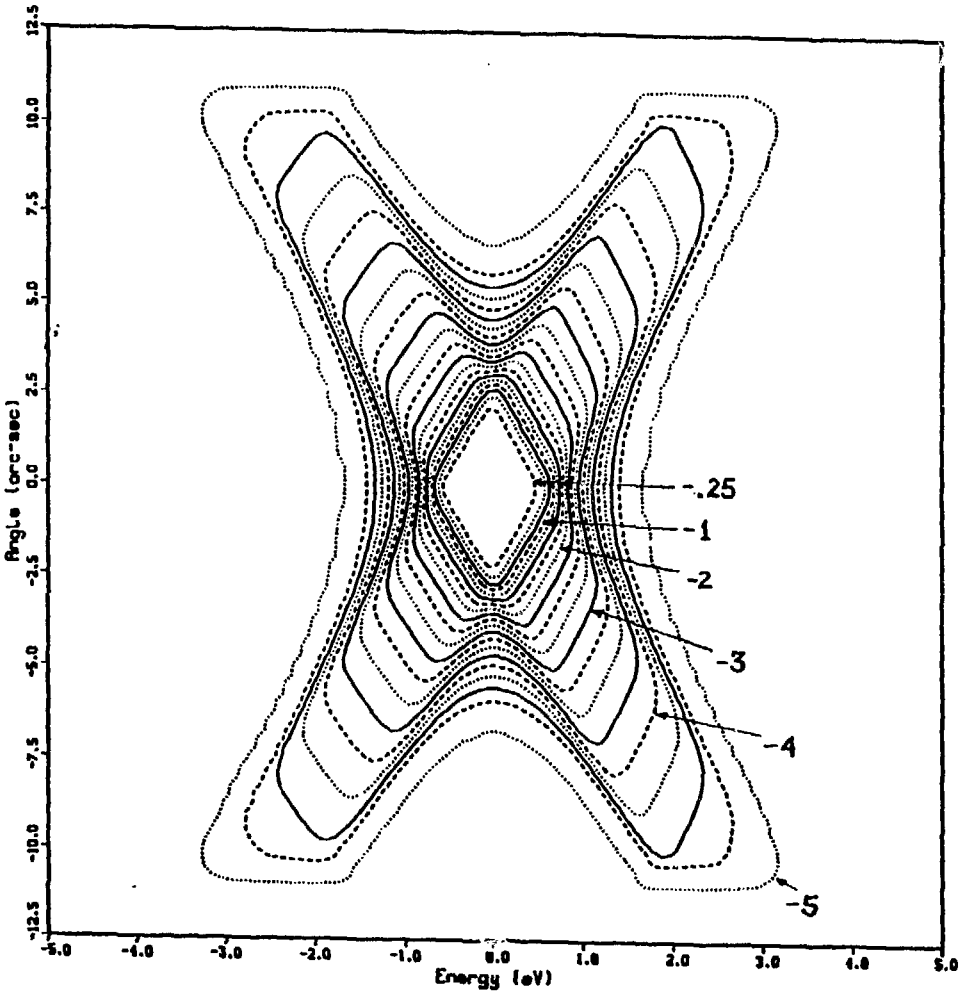

Thruput
Relative Energy (eV)
Relative Angle (arc-sec)


Thruput
Relative Energy (eV)
Relative Angle (arc-sec)


Angle (arc-sec)
12.5
10.0
7.5
5.0
2.5
0.0
-2.5
-5.0
-7.5
-10.0
-12.5
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
5.0
Energy (eV)
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-1
-2
-3
-4
-5