The Toroidal Grating Monochromator at Beam Line 8-1

March 16, 2000

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1. Introduction

The toroidal grating monochromator (TGM) at beam line 8-1 was installed in 1986 by a collaboration between SSRL and LLNL. The purpose of this document is to provide the reader with an understanding of the beam line's capabilities and shortcomings. In addition the reader is provided with an explanation of why the beam line is the way it is. Hopefully this will be of some use to the initiate as well as to those with many years of experience.

2. Beam Line Optics

2.1 M0 Mirror

The M0 mirror is a platinum coated CVD-SiC cylinder that deflects and focuses 12 mrad horizontally onto the entrance slit. The mirror intercepts the beam at an angle of 6° yielding the reflectivity curve in Figure 1. The mirror is located at 8.5 m from the source and collects three mrad in the vertical. The mirror measures 3.5 cm thick, 11 cm wide and 30 cm long (Figure 2). The radius of curvature is 92.5 cm in the saggital, which provides a horizontal focus at 18m from the source (at the location of the entrance slit).

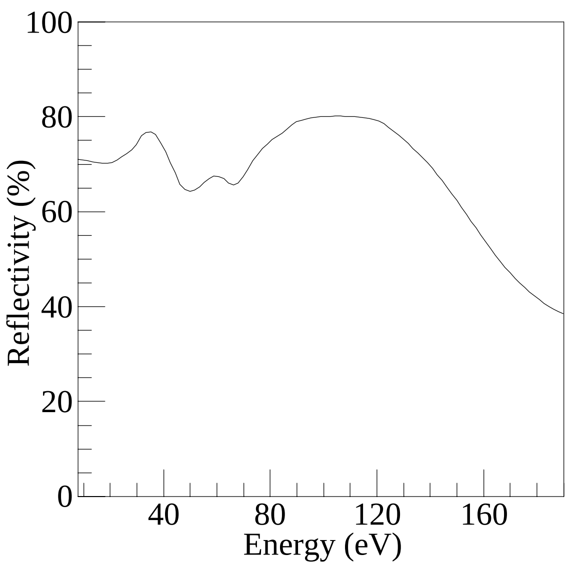

Figure 1 Platinum Reflectivity at 6°

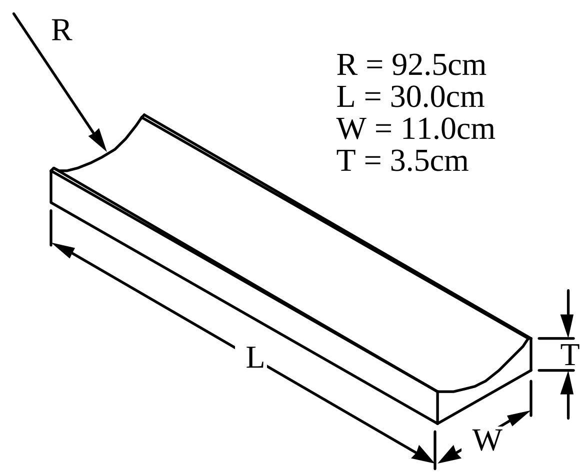

Figure 2 Mirror Dimensions

The radius of curvature required for focusing given the image distance i, object distance o and angle of incidence θ, can be derived from the following equation(Figure 3):

$$\frac{1}{o} + \frac{1}{i} = \frac{1}{f}$$

Where

$$f = \frac{R}{2\sin\theta}$$

for the horizontal focal point.

Solving for R we have:

$$R_H = \frac{2io\sin\theta}{i+o}.$$

The mirror position is controlled manually by stepper motor with encoder read back. The motions available are vertical translation and tilt and horizontal translation and rotation.

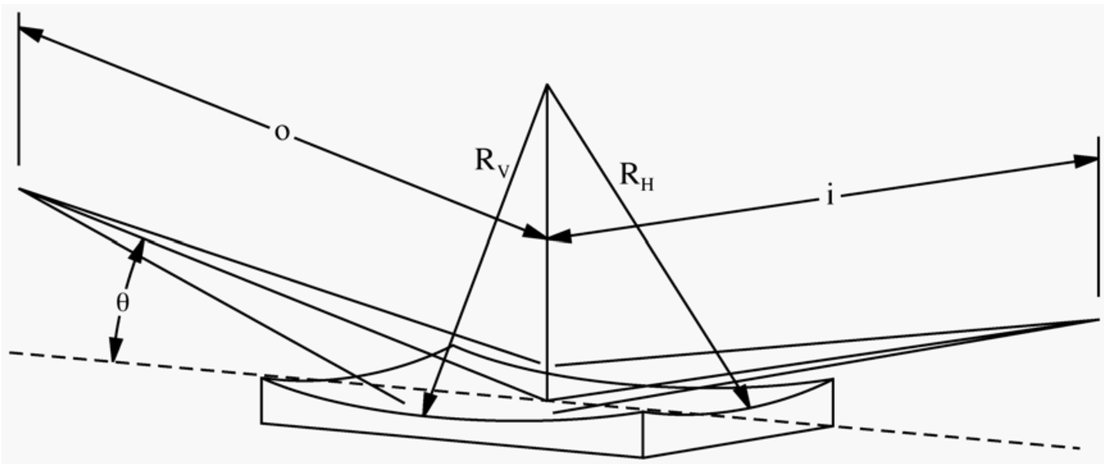

Figure 3 Mirror Nomenclature

2.2 M1 Mirror

The M1 mirror is a platinum coated spherical mirror that deflects and focuses the beam vertically onto the entrance slit and also intersects the beam at an angle of 6° -- with a reflectivity curve as seen in Figure 1. The mirror is located 13 m from the source and measures 4.5 cm thick, 8.1 cm wide and 45.2 cm long. The radius of curvature is 6.3654 m, which provides a focus in the vertical at 18m from the source.

The radius of curvature required for focusing given the image distance i, object distance o and angle of incidence θ, can be derived from the above equation where

$$f = \frac{R\sin\theta}{2}$$

for the vertical focal point. Solving for R we have:

$$R_v = \frac{2io}{(i+o)\sin\theta}$$

2.3 Entrance Slit

The entrance slit is adjustable from 10 to 100 µm in the vertical, and from 5 mm to 20 mm in the horizontal in 5 mm steps. It is located 18 meters from the source.

2.4 Monochromator

The monochromator is built around a set of three toroidal gratings. The gratings have a line spacing of 288, 822 and 2400 l/mm. This gives the monochromator an energy range of 8 - 200 eV.

2.4.1 Grating Diffraction

The grating equation can be derived from the optical path function with the constraint that the photons can only travel a path that varies by discrete values because of the periodicity of the grating (see appendix 1). From the optical path function the grating equation is written as

$$m\lambda = d\,(\sin\alpha + \sin\beta)$$

Where m is the order, d is the groove to groove distance in angstroms, λ is the wavelength, and α and β are the input and output angles of the photon (see Figure 4).

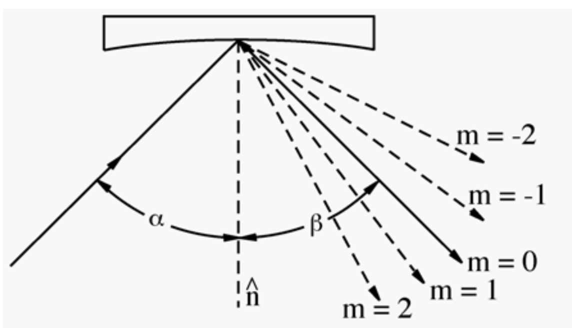

Figure 4 Grating Nomenclature

The angle that the entrance and exit slits make with respect to the grating is a constant ϕ and is referred to as the opening angle of the monochromator. Using the sign convention that positive angle is expressed as the clockwise direction from the normal and that angles on opposite sides of the normal have opposite signs allows us to express ϕ as a function of α and β:

$$\phi = \alpha - \beta$$

thus the sum of α and β are constant.

The zero order position is the position of the grating where the grating behaves as a mirror. By the law of reflection the magnitudes of α and β must be equal and are one-half the opening angle ϕ.

Knowing ϕ allows us to solve for α as a function of λ as follows:

$$m\lambda = d\,(\sin\alpha + \sin\beta)$$

$$m\lambda = d(2\sin\frac{1}{2}(\alpha+\beta)\cos\frac{1}{2}(\alpha-\beta))$$

$$\frac{m\lambda}{2d} = \sin(\alpha - \frac{\phi}{2})\cos\frac{\phi}{2}$$

$$\sin(\alpha - \frac{\phi}{2}) = \frac{m\lambda}{2d\cos\frac{\phi}{2}}$$

$$\alpha = \arcsin\left(\frac{m\lambda}{2d\cos\frac{\phi}{2}}\right) + \frac{\phi}{2}$$

and since $\beta = \alpha - \phi$

$$\beta = \arcsin\left(\frac{m\lambda}{2d\cos\frac{\phi}{2}}\right) - \frac{\phi}{2}.$$

Energy is related to wavelength by the function

$$E = \frac{h\nu}{\lambda}$$

where $h\nu$ is 12398.4244 eV-Å and d is related to N, the number of grooves per millimeter by

$$d(\ \ ) = \frac{1}{N}\left(\frac{mm}{g}\right)\left(10^{7}\frac{\ }{mm}\right)$$

α and β as a function of energy and grooves per millimeter are now

$$\alpha = \arcsin\left(\frac{mh\nu N\cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right) + \frac{\phi}{2}$$

$$\beta = \arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right) - \frac{\phi}{2}$$

where E is in eV.

2.4.2 Horizon Wavelength

The horizon wavelength is the longest wavelength (and thus lowest energy) that can be diffracted by the grating and occurs when alpha or beta is at 90°. Solving the grating equation for wavelength gives us in first order:

$$\frac{\lambda_H}{2d} = \sin(90 + \frac{\phi}{2})\cos\frac{\phi}{2}$$

$$\lambda_H = 2d\cos(-\frac{\phi}{2})\cos\frac{\phi}{2}$$

$$\lambda_H = 2d\cos^2\frac{\phi}{2}$$

$$\lambda_H = \frac{2 \cdot 10^7}{N}\cos^2\frac{\phi}{2}$$

The horizon wavelengths for the 3 gratings installed in 8-1 are in Table 1

N	λ_H(Å)	E(eV)
288	2094.00	5.921
822	733.67	16.899
2400	251.28	49.34

Table 1 Horizon Wavelengths

2.4.3 Tangential Radius of Curvature R

Given that we want to maximize the slit to slit distance, L, to the extent of the space available, the radius of curvature R for the meridian focus can be determined from Figure 5:

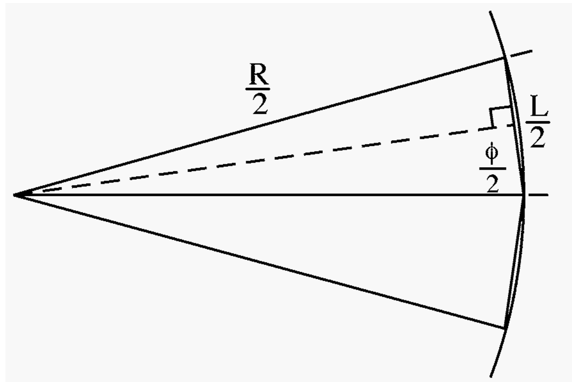

Figure 5 Tangential Radius of Curvature

Since we have constrained the slits and the grating to lie on the Rowland circle and the Radius of curvature of the grating must be twice the radius of the Rowland circle we have:

$$\frac{L}{2} = 2\frac{R}{2}\cos\left(\frac{\phi}{2}\right)$$

and solving for R yields

$$R = \frac{L}{2\cos\left(\frac{\phi}{2}\right)}$$

Given an opening angle ϕ of 160° and a nominal slit to slit distance of 6m R is found to be 19.224 m. This number is somewhat arbitrary and acts as an overall scale factor for the monochromator. R plays a large part in the resolutions and is used to determine the optimal position of the exit slit.

2.4.4 Saggital Radius of Curvature ρ

The saggital or horizontal radius of curvature is determined by setting the equation for astigmatism (see appendix 1) to zero and solving for ρ as follows:

$$F_{02} = z^2\left(\frac{1}{r_a} - \frac{\cos\alpha}{\rho} + \frac{1}{r_b} - \frac{\cos\beta}{\rho}\right) = 0$$

where z is the half width of the grating, r_a and r_b are the entrance and exit slit distances and α and β are the incidence and diffraction angles. Solving for ρ:

$$\rho = \frac{r_a r_b(\cos\alpha + \cos\beta)}{r_a + r_b}$$

This equation does not give us a unique radius of curvature but is dependent upon α and β and thus the energy of the photon. If we examine the sum $\cos\alpha + \cos\beta$ for the particular case of the 288 l/mm grating we see that the it changes very little with respect to energy (Table 2).

eV	α	β	cosα+cosβ
10	85.9013	-74.0957	.3455
20	82.9467	-77.0533	.3468
30	81.9640	-78.0360	.3471

Table 2 cosα + cosβ

This shows that if we select a radius of curvature that is optimized for the middle of the energy range, this radius will place the astigmatism close to zero for the entire range.

For a nominal entrance slit distance of 2111 mm and exit slit distance of 3888 mm we can calculate ρ to be 474 mm.

2.4.5 Resolution

The resolution of the monochromator is the vector sum of the resolutions from the slit widths, diffraction limit, aberrations and slope error.

2.4.5.1 Slit Width Resolution

For a fixed input angle α we can differentiate the grating equation and find the angular dispersion:

$$\lambda = \frac{d(\sin\alpha + \sin\beta)}{m}$$

$$\mathbf{d}\lambda = \frac{d\cos\beta}{m}\mathbf{d}\beta$$

Given the angular dispersion, the reciprocal linear dispersion can be calculated (Figure 6):

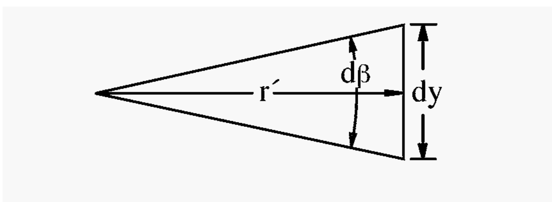

Figure 6 Reciprocal Linear Dispersion

$$\frac{\mathbf{d}y}{2} = r_b \tan\frac{\mathbf{d}\beta}{2}$$

For small angles this reduces to

$$\mathbf{d}y = r_b\mathbf{d}\beta.$$

The reciprocal linear dispersion is thus

$$\mathbf{d}\lambda = \frac{d\cos\beta}{r_b m}\mathbf{d}y$$

and for a fixed β

$$\mathbf{d}\lambda = \frac{d\cos\alpha}{r_a m}\mathbf{d}y$$

The slit width resolutions are found by substituting the slit opening for **d**y:

$$\Delta\lambda_{S1} = \frac{S_1 d\cos\alpha}{r_a m}$$

$$\Delta\lambda_{S2} = \frac{S_2 d\cos\beta}{r_b m}$$

Converting d to N and using the values of S in microns, r in meters and N in l/mm we have in units of Å:

$$\Delta\lambda_{S1} = 10\frac{S_1\cos\alpha}{r_a mN}$$

and

$$\Delta\lambda_{S2} = 10\frac{S_2\cos\beta}{r_b mN}$$

2.4.5.2 Diffraction Limited Resolution

The diffraction limited resolution is defined as:

$$\Delta\lambda_D = \frac{\lambda}{mn}$$

where n is the number of grooves participating in the diffraction process.

2.4.5.3 Aberration Resolutions

The resolutions resulting from the various aberrations are defined as follows:

$$\Delta\lambda_{ijk} = \frac{d}{m}\left(\frac{\partial F_{ijk}}{\partial y}\right)$$

Where F_{ijk} is the aberration term as derived from the expansion of the optical path function (see appendix 1).

The terms with which we are primarily concerned are defocus (F_{200}) coma (F_{300}) and astigmatic coma (F_{120}). Performing the derivatives we find

$$\Delta\lambda_{200} = \frac{dy}{m}\left(\frac{\cos^2\alpha}{r_a} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{r_b} - \frac{\cos\beta}{R} + \frac{\cos^2\gamma}{r_c} - \frac{\cos\gamma}{R} + \frac{\cos^2\delta}{r_d} - \frac{\cos\delta}{R}\right)$$

$$\Delta\lambda_{300} = \frac{3dy^2}{m}\left[\begin{array}{l}\left(\frac{\cos^2\alpha}{r_a} - \frac{\cos\alpha}{R}\right)\frac{\sin\alpha}{2r_a} + \left(\frac{\cos^2\beta}{r_b} - \frac{\cos\beta}{R}\right)\frac{\sin\beta}{2r_b} \\ + \left(\frac{\cos^2\gamma}{r_c} - \frac{\cos\gamma}{R}\right)\frac{\sin\gamma}{2r_c} + \left(\frac{\cos^2\delta}{r_d} - \frac{\cos\delta}{R}\right)\frac{\sin\delta}{2r_d}\end{array}\right]$$

and

$$\Delta\lambda_{120} = \frac{dz^2}{m}\left[\left(\frac{1}{r_a} - \frac{\cos\alpha}{\rho}\right)\frac{\sin\alpha}{2r_a} + \left(\frac{1}{r_b} - \frac{\cos\beta}{\rho}\right)\frac{\sin\beta}{2r_b} + \left(\frac{1}{r_c} - \frac{\cos\gamma}{\rho}\right)\frac{\sin\gamma}{2r_c} + \left(\frac{1}{r_d} - \frac{\cos\delta}{\rho}\right)\frac{\sin\delta}{2r_d}\right]$$

where y and z are the dimensions of the illuminated portion of the grating in the tangential and saggital directions.

2.4.5.4 Slope Error Resolution

The resolution component due to the slope error is defined as:

$$\Delta\lambda_\sigma = 2\sigma\cot\psi$$

where σ is the slope error in radians and

$$\psi = \arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right).$$

2.4.5.5 Total Resolution

The total resolution is the vector sum of the various resolutions.

$$\Delta\lambda = \sqrt{\Delta\lambda_{S1}^2 + \Delta\lambda_{S2}^2 + \Delta\lambda_D^2 + \Delta\lambda_{200}^2 + \Delta\lambda_{300}^2 + \Delta\lambda_{120}^2 + \cdots}.$$

The resolution of 8-1 for the various contributors is shown in Figure 7 for the 288 l/mm grating with entrance and exit slits set at 10 μm, 1μrad slope error and vertical and horizontal acceptances of 75 by 10 mm. Similar conditions for the 822 and 2400 l/mm gratings are shown in Figure 8 and Figure 11.

The total resolution as a function of slit size is shown for each grating at 10, 50 and 100 μm in Figure 9, Figure 10 and Figure 12:

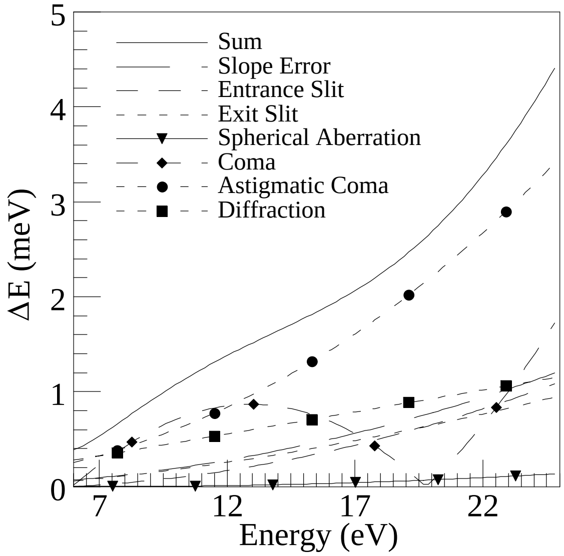

Figure 7 288 l/mm Resolution

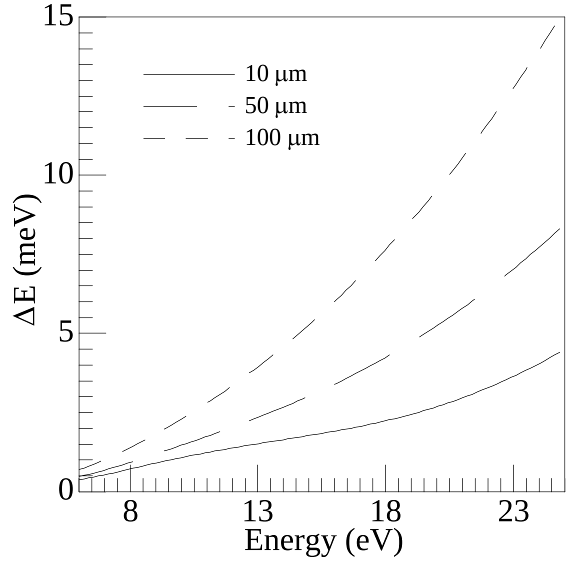

Figure 9 288 l/mm Slit Resolutions

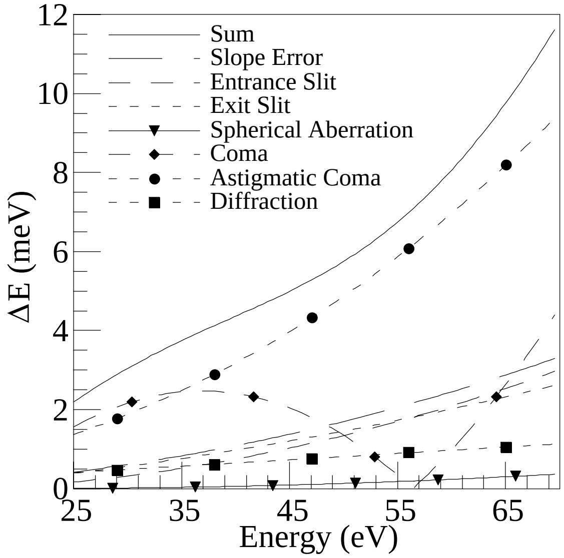

Figure 8 822 l/mm Resolution

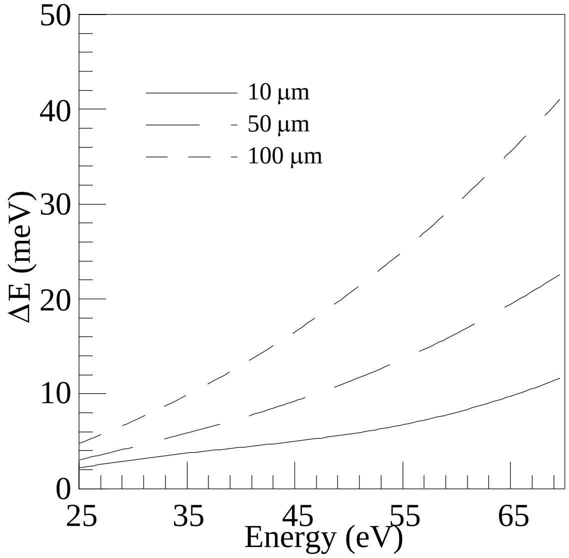

Figure 10 822 l/mm Slit Resolutions

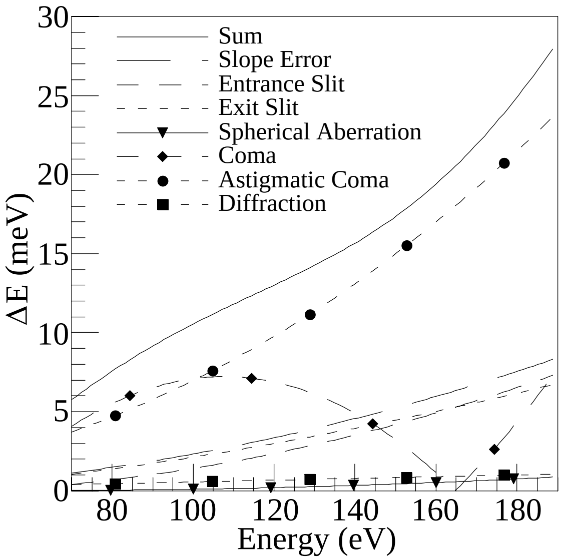

Figure 11 2400 l/mm Resolution

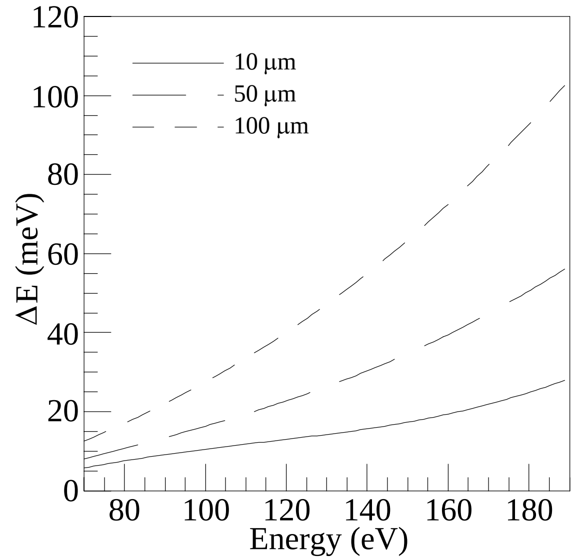

Figure 12 2400 l/mm Slit Resolutions

2.4.6 Grating Efficiencies

The efficiency of a phase amplitude grating can be calculated given 100% reflectivity by the following formula for odd orders:

$$E_m = \frac{400}{m^2\pi^2}\sin^2\frac{1}{2}\delta'$$

where

$$\delta' = \left(\frac{2\pi}{\lambda}\right)h(\cos\alpha + \cos\beta)$$

In the preceding two equations m is the order, λ is the wavelength, α and β are the angles of diffraction and h is the depth of the grooves (see appendix 2). The optimal groove depth h as a function of wavelength can be determined from:

$$h = \frac{1}{\sqrt{\frac{8\sin\alpha}{\lambda d}m + \frac{1}{h_0^{\,2}}} + \frac{1}{h_0}}$$

where

$$h_0 = \frac{\lambda}{2\sin\alpha}$$

For 8-1 the optimal groove depths are given in Table 3

Grating	Energy	Groove Depth (Å)

288	20	891.8514
822	55	324.2976
2400	125	142.6526

Table 3 Groove Depths

Given the optimum groove depths for the various gratings we can now plot the efficiency for each grating as a function of energy (Figure 13 through Figure 15).

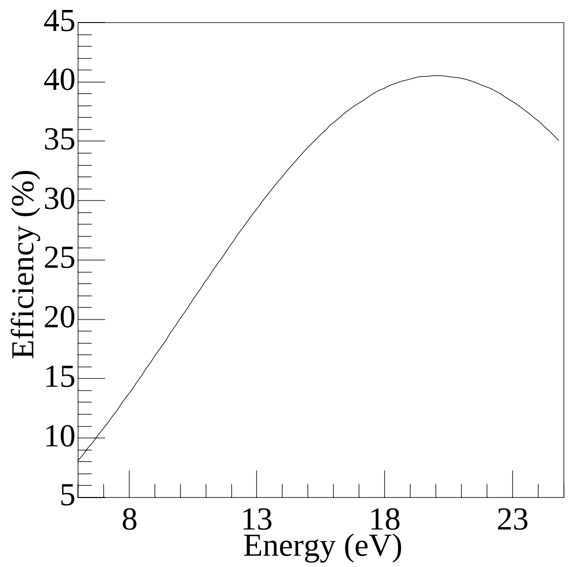

Figure 13 288 l/mm Scalar Efficiency

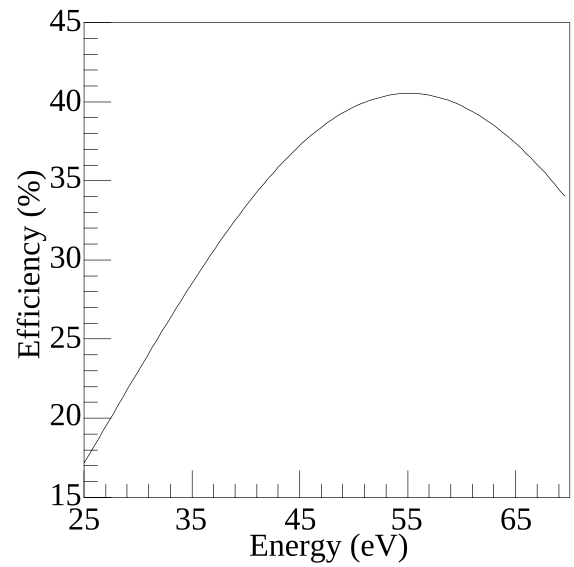

Figure 14 822 l/mm Scalar Efficiency

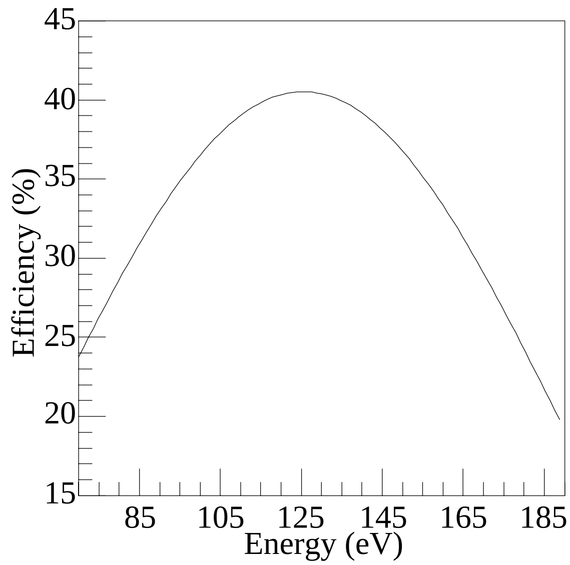

Figure 15 2400 l/mm Scalar Efficiency

2.4.7 Performance

Multiplying the efficiencies of the M_0 mirror, M_1 mirror, gratings and refocussing mirror will give us an overall picture of the theoretical performance of the beam line.

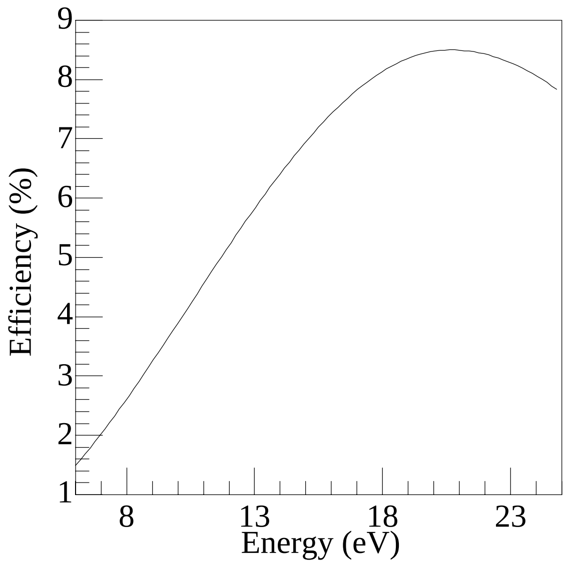

Figure 16 288 l/mm Total Efficiency

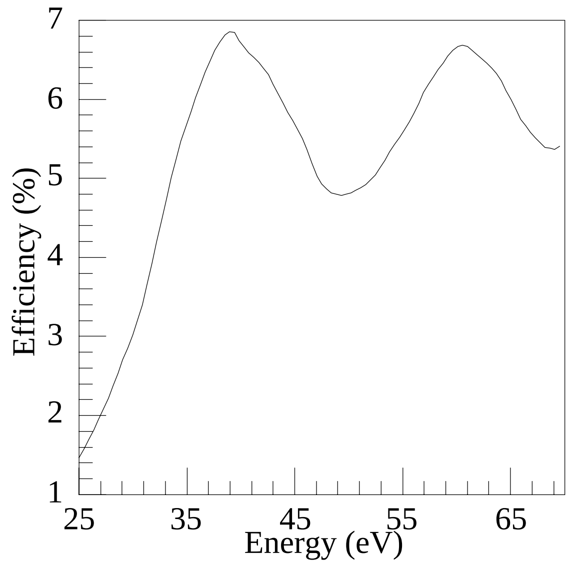

Figure 17 822 l/mm Total Efficiency

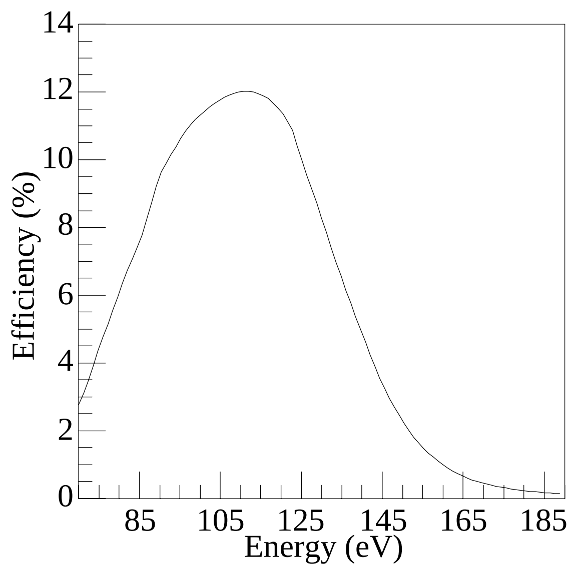

Figure 18 2400 l/mm Total Efficiency

2.4.8 Monochromator Mechanics

The grating rotation is achieved by pushing on a sin-bar with a slide and stepper motor. The linear position of the slide as a function of the desired angle δ and sin-bar length l plus some arbitrary starting position x is (Figure 19)

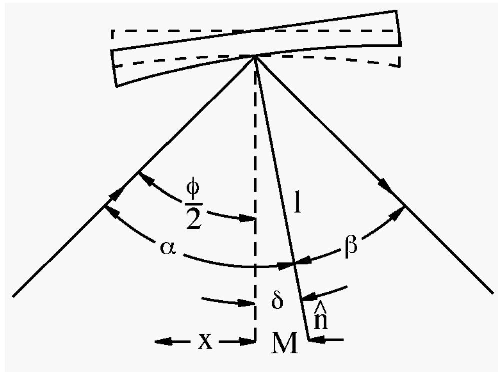

Figure 19 Sin-bar Nomenclature

$$M = x + l\tan\delta.$$

From Figure 19 δ is

$$\delta = \alpha - \frac{\phi}{2}$$

and

$$M = x + l\tan\left(\alpha - \frac{\phi}{2}\right)$$

substituting for α yields

$$M = x + l\tan\left[\arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right)\right].$$

If we position the slide at the zero order position of the grating (M = zop) and use the fact that at the zero order position

$$\alpha = \frac{\phi}{2}$$

we have

$$\frac{\phi}{2} = \arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right) + \frac{\phi}{2}$$

$$\arcsin\left(\frac{mh\nu N\cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right) = 0$$

and solving for x we have

$$x = zop.$$

Finally we have a complete expression for the position of the slide given the desired energy E, and measured zero order position zop:

$$M = zop + l\tan\left[\arcsin\left(\frac{mh\nu N\cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right)\right]$$

Conversely we can solve the above equation for energy E:

$$E = \frac{mh\nu N\cdot 10^{-7}}{2\cos\frac{\phi}{2}\sin\left(\arctan\left(\frac{zop - M}{l}\right)\right)}$$

These last two equations are the geometrical forward and backward transfer equations for the 8-1 TGM. The parameters for these equations are given in Table 4

Parameter	Value
φ	160°
l	381000 steps
m	1

Table 4 8-1 Parameters

Given that we can nominally calibrate the grating by finding the zero order position and then using that to fix our angle and hence energy, this calibration is rarely accurate. To fix the monochromator position to a known energy, we can shift the zero order position so that there is agreement between them. If we have two positions M_m and M_a for the positions of the measured and actual energies of a calibration feature and we let $f(E_m)$ and $f(E_a)$ be our ltan() terms we can rewrite our transfer functions as follows

$$M_m = zop_m + f(E_m)$$

and

$$M_a = zop_a + f(E_a).$$

We want M_m and M_a to be equal so that

$$M_m = zop_a + f(E_a).$$

Solving for zop_a:

$$zop_a = M_m - f(E_a).$$

However M_a is really a function of zop_m so that

$$M_a = zop_m + f(E_a)$$

and solving for $f(E_a)$ and substituting it into our expression for zop_a yields

$$zop_a = zop_m + M_m - M_a.$$

This expression allows us to calibrate the monochromator now to any single energy.

2.4.9 Monochromator Approximation

The geometrical transfer equations allow us to move the monochromator to any energy, but the calibration of that energy can only be modified by changing the zero order position. Although we could change the dispersion by changing the value for the number of lines per millimeter, this is a very difficult adjustment to get right.

An easier method is to fix the dispersion by fitting a second order polynomial to two energies and the zero order position. This leaves us with the two energies we have chosen at the exact positions we desire.

Obviously the units of our three points are not the same, so we want to relate them to each other in a sensible manner. Using electron volts as our units puts the zero order position at infinity, but using a function of α or β leaves us with nice rational numbers to calculate our polynomial.

If we define

$$\psi = \beta - \frac{\phi}{2}$$

we have

$$\psi = \arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right)$$

and for the zero order position where

$$\beta = \frac{\phi}{2}$$

we have $\psi = 0$.

Assigning ψ_N to the zero order position, energy one and energy two, we can generate three simultaneous equations :

$$C_0 + C_1\psi_N + C_2\psi_N^2 = S_N$$

where the C_N are the coefficients for the calibration and the S_N are the positions of the slide for our three points.

In matrix form we have

$$\begin{bmatrix} \psi_0^2 & \psi_0 & 1 \\ \psi_1^2 & \psi_1 & 1 \\ \psi_2^2 & \psi_2 & 1 \end{bmatrix} \begin{bmatrix} C_2 \\ C_1 \\ C_0 \end{bmatrix} = \begin{bmatrix} S_0 \\ S_1 \\ S_2 \end{bmatrix}.$$

Applying Cramers rule we have for

$$\mathbf{Ax} = \mathbf{B}$$

the solution

$$x_i = \frac{\text{Det}\mathbf{A}_i}{\text{Det}\mathbf{A}}$$

Where $\mathbf{A}_i$ is obtained by replacing the ith column of **A** with **B**.

The above solutions determine the coefficients for an absolute calibration, one where the energies and zero order position are know with respect to their slide positions. If we want to change the calibration by referring an old energy to a new energy we must generate a new matrix and again apply Cramers rule.

Let $E_{1,2}$ be the energies of the current calibration with the appropriate $\psi_{1,2}$ and $S_{1,2}$, and use primed notation for the corrected calibration. The corrected $\psi'_{1,2}$ should then be paired with the current calibration $S_{1,2}$ and the current ψ_0 should be paired with the corrected S'_0 (remember that our angle for the zero order position never changes). Our new matrix is now

$$\begin{bmatrix} \psi_0^2 & \psi_0 & 1 \\ \psi'^2_1 & \psi'_1 & 1 \\ \psi'^2_2 & \psi'_2 & 1 \end{bmatrix} \begin{bmatrix} C_2 \\ C_1 \\ C_0 \end{bmatrix} = \begin{bmatrix} S'_0 \\ S_1 \\ S_2 \end{bmatrix}$$

with solutions found by applying Cramers rule.

Our new calibrated forward transfer equation is now

$$S = C_0 + C_1\psi + C_2\psi^2$$

with

$$\psi = \arcsin\left(\frac{mh\nu N \cdot 10^{-7}}{2E\cos\frac{\phi}{2}}\right).$$

Our backward transfer equation is found by solving for ψ and then E. Using the solution of the quadratic equation we have

$$\psi = \frac{-C_1 + \sqrt{C_1^{\,2} - 4C_2(C_0 - S)}}{2C_2}$$

and

$$E = \frac{mh\nu N \cdot 10^{-7}}{2\cos\frac{\phi}{2}\sin\left(\frac{-C_1 + \sqrt{C_1^{\,2} - 4C_2(C_0 - S)}}{2C_2}\right)}$$

2.5 Exit Slit

The exit slit consists of vertical and horizontal apertures that are adjustable from 10 µm to 2mm in the vertical and 100µm to 20 mm in the horizontal. The slit assembly can be translated along the beam direction over a range of 500mm. The optimal position of the exit slit is determined by setting the defocus term to zero and solving for r´ as follows:

$$F_{200} = \frac{\cos^2\alpha}{r_a} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{r_b} - \frac{\cos\beta}{R} + H = 0$$

where α, β, r_a, r_b, and R are as defined previously and H is the contribution to the defocus term due to the holographic nature of the gratings (see appendix 1):

$$H = \frac{m\lambda}{\lambda_0}\left(\frac{\cos^2\gamma}{r_c} - \frac{\cos\gamma}{R} + \frac{\cos^2\delta}{r_d} - \frac{\cos\delta}{R}\right)$$

With λ and λ_0 the wavelength of interest and laser wavelength respectively.

Now

$$r_b = \frac{Rr_a \cos^2 \beta}{r_a(\cos\beta + \cos\alpha) - R\cos 2\beta + Rr_a H}.$$

Using the parameters given in Table 5 we can plot the location of the exit slit for the three gratings versus energy (Figure 20, Figure 21, and Figure 22) and wavelength (Figure 23, Figure 24, and Figure 25). The positions of the exit slit are also tabulated in appendix 2.

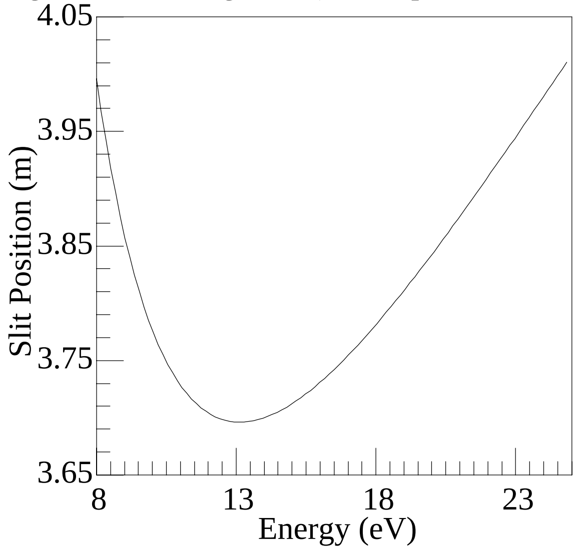

Figure 20 Exit Slit Position for 288 l/mm grating

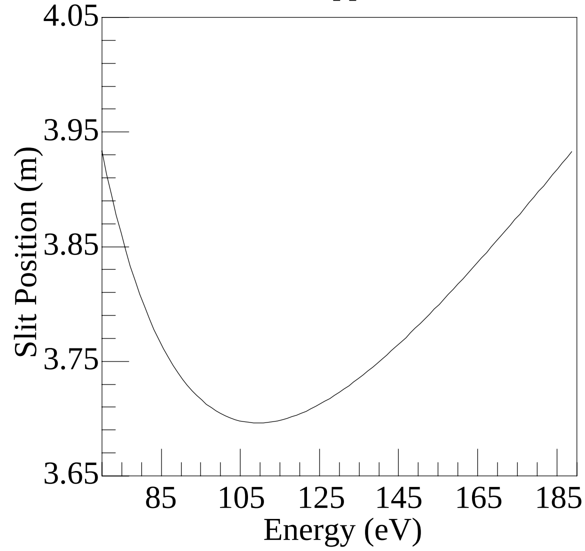

Figure 22 Exit Slit Position 2400 l/mm grating

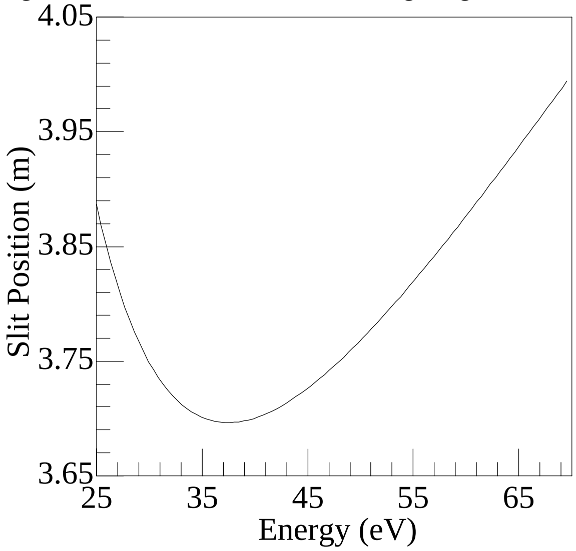

Figure 21 Exit Slit Position for 822 l/mm grating

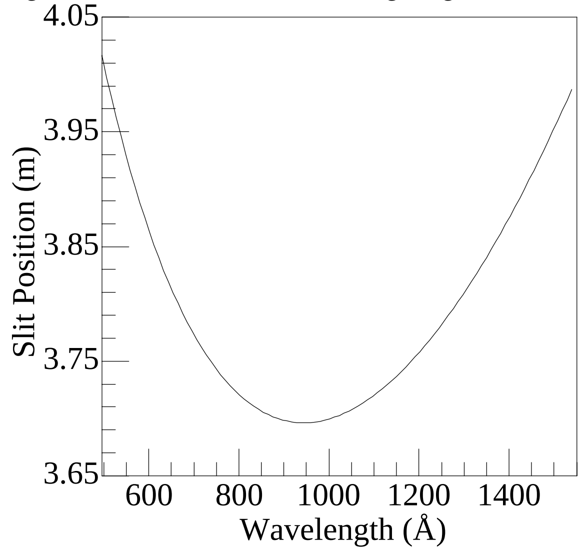

Figure 23 Exit Slit Position 288l/mm grating

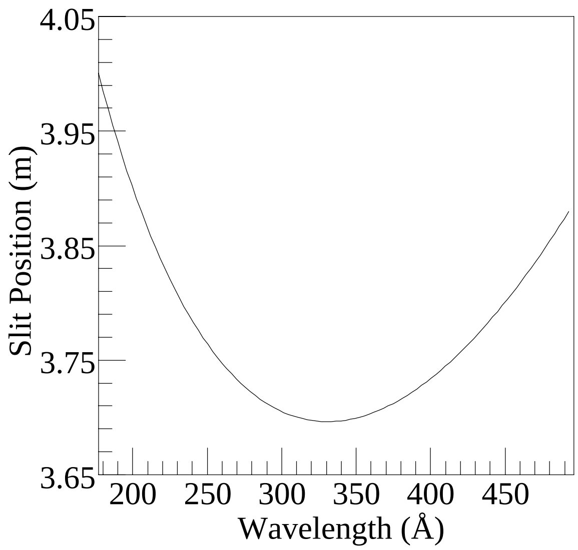

Figure 24 Exit Slit Position 822 l/mm grating

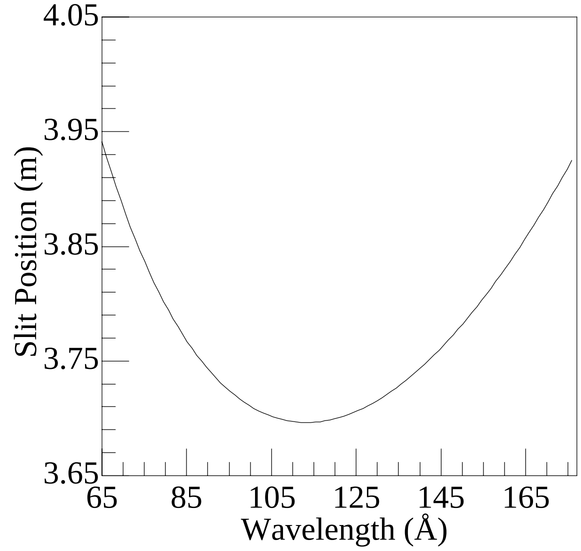

Figure 25 Exit Slit Position 2400 l/mm grating

N	γ	δ	$\mathbf{r_C}$	$\mathbf{r_D}$
288	3.78°	3.78°	16.623 m	16.623 m
822	10.84°	10.84°	13.054 m	13.054 m
2400	33.33°	33.33°	6.344 m	6.344 m

Table 5 Holographic Grating Parameters

2.6 Filters

Downstream of the exit slit are a set of filters that are mounted on a linear feed through. The filters their thickness’, and their positions are described in Table 6.

Filter	**Thickness**	**Position**
In:Ti	1600Å	996.45
Mo	1000Å	6.45
Sn:Ge	1600Å	16.3
Al	1500Å	26.7
Si	1500Å	36.26
B	3000Å	46.1
C	1000Å	56.76

Table 6 Filters

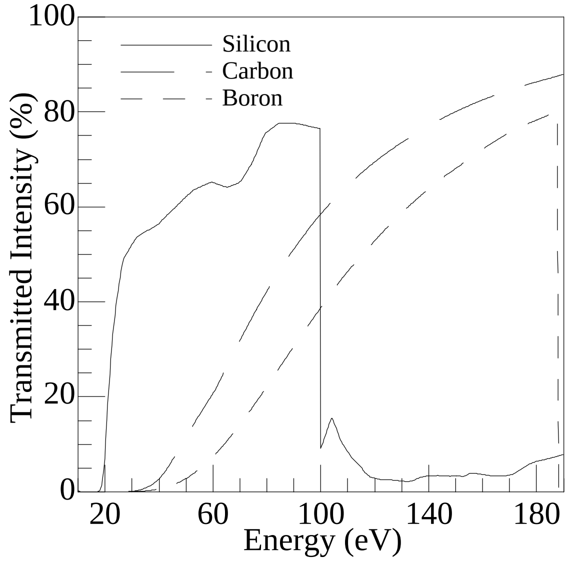

Figure 26 Silicon, Carbon, and Boron Filters

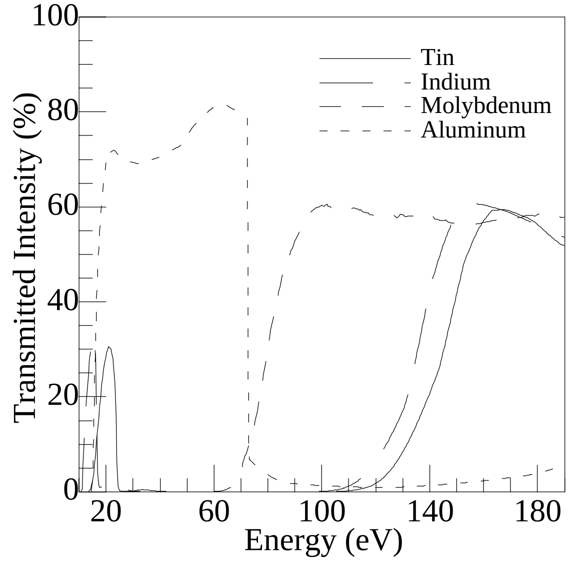

Figure 27 Tin, Indium, Moly, and Aluminum Filters

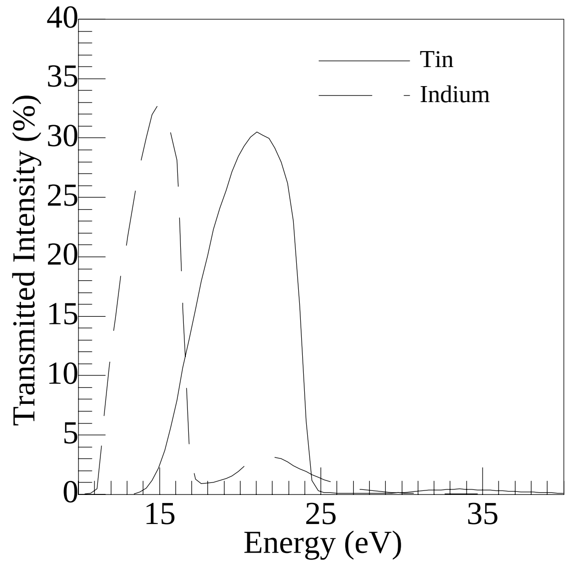

Figure 28 Tin and Indium Filters

2.7 Refocussing Mirror

The final mirror in the beam line is the refocussing mirror. This mirror is a platinum coated bendable cylinder located 3 meters from its source point and 1 meter from its image point. The mirror intercepts the beam at an angle of 2° with a resulting reflectivity in figurex. Given o = 3, i =1 and θ = 2° the radius of curvature ρ is 5.2 cm (see section 2.1).

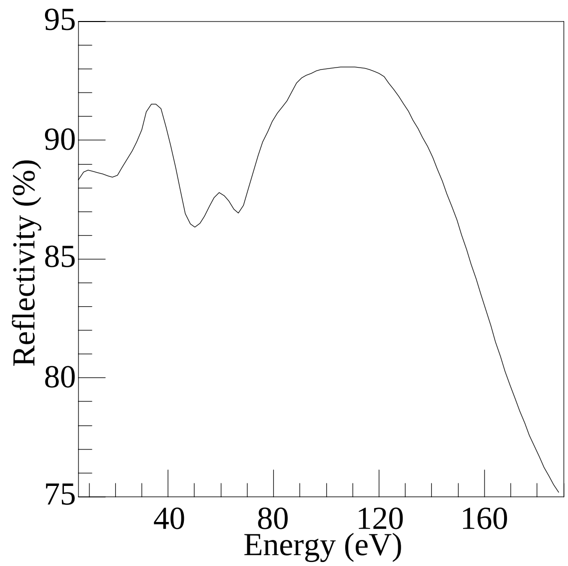

Figure 29 Refocusing Mirror Reflectivity

The mirror can be adjusted in tilt and yaw via three independant micrometers that are mounted out of vacuum.

2.8 I_0 Section

The I_0 section is equipped with a gold grid from which either the photo emitted current can be measured directly or the photo current can be amplified via a channeltron and battery box/Fluke high voltage power supply which is supplied. There is also a set of baffles that allow both vertical and horizontal aperturing of the beam.

3. Beam Line Electronics

The beam line electronics consists of the motion control system and the data acquisition system.

3.1 Motion Control System

The motion of the monochromator is achieved through the use of Compumotor SX indexer-drivers with encoder feedback. These indexers are connected to the RS232 serial port of an Alpha workstation. The indexers operate in closed loop encoder mode. The motor resolutions are 25000 steps per revolution, and the encoder resolutions are 640 and 205 steps per revolution for the grating and exit slit respectively.

To set up the indexers log into the system using a privileged account such as STEWARDS and give your process all privileges. Then at the prompt type

```
81STEW>set host ttb0:/dte
```

The alpha will then connect to the indexer and respond with the following:

```
%REM-I-TOQUIT, connection established
```

```
Press Ctrl/\ to quit, Ctrl/@ for command mode
```

At this point you are communicating with the indexer directly. The command to query the indexer as to its status is the ID number followed by DR and a space. For 8-1 the ID number is one for the exit slit and two for the grating. The indexers should respond to the query with the following:

```
1DR *SX_SETTINGS*
*CONFIGURED_AS_A_INDEXER
*MOTION_MODE:_INCREMENTAL_PRESET
*0__CW_AND_CCW_LIMITS_ENABLED
*3__NO_SOFTWARE_TRAVEL_LIMITS_ENABLED
*MOTION_PARAMETERS:*A1.0   *AD1.0   *V1.0   *D-10
*SET_UP_PARAMETERS:*MR11____25000_STEPS_PER_REV
                   *ER205
*____SOFTWARE_SWITCHES_____*
*___ABCD_EFGH_IJKL_MNOP_QRST
*SS*0000_0000_1000_0100_0000
*FS*0100_0000_0000_0000
*OS*0111_0000_00
```

for number one and:

```
2DR *SX_SETTINGS*
*CONFIGURED_AS_A_INDEXER
*MOTION_MODE:_INCREMENTAL_PRESET
*0__CW_AND_CCW_LIMITS_ENABLED
*3__NO_SOFTWARE_TRAVEL_LIMITS_ENABLED
*MOTION_PARAMETERS:*A1.0   *AD1.0   *V1.0   *D-4735
*SET_UP_PARAMETERS:*MR11____25000_STEPS_PER_REV
                   *ER640
*____SOFTWARE_SWITCHES_____*
*___ABCD_EFGH_IJKL_MNOP_QRST
*SS*0000_0000_1000_0100_0000
*FS*0100_0000_0000_0000
*OS*0111_0000_00
```

for number two.

The important things to verify are the motor resolution, the encoder resolution and the SS and FS status flags. These items should be exactly as they appear above. Table 7 contains the commands for setting the indexers properly. Note that all commands should be followed with a space in order to execute.

Exit Slit	**Grating**	**Description**
1MR11	2MR11	Sets the motor resolution to 25000
1ER205	2ER640	Sets the encoder resolution to 205 and 640 steps
1SSI1	2SSI1	Disable interactive mode
1FSB1	2FSB1	Set indexer to encoder step mode

Table 7 Indexer Commands

After these items have been set properly type control\ and the system will respond with:

```
%REM-S-END, control returned to node S081
```

3.2 Data Acquisition System

The data acquisition system consists of an Alpha work station and a CAMAC crate. Data acquisition can be controlled by either SUPER or XAS working through the interface package ICS. Both packages can read multiple hex-scalars and scan the monochromator. Both systems complement each other in that SUPER allows the user to control multiple devices in complex ways (CMA's for example) but only allows up to three energy regions to be scanned, while XAS can scan a very large number of energy regions but can only really control the monochromator.

For data collection there are installed a set of six hex scalars and 4 V-F converters. This is adequate for most users but it is possible to install more if required. Also provided is a pair of digital to analog converters for the control of a CMA.

4. Software

The monochromator is controlled by ICS. ICS is the interface software between the higher level data acquisition programs SUPER and XAS, and the CAMAC crate and other external devices. This software has utilities for starting the system, manipulating the motors and devices in the CAMAC crate, and detailed control of the individual motors. The motion of the monochromator is determined by a program written in the ICS pseudo-code. This program allows the user to move the monochromator in energy using either the geometrical transfer equations or the calibrated transfer equations. A complete listing of the code is given in appendix 3.

4.1 ICS_CPC

This utility starts and stops the control system and the control system should be shut down before any modifications are made to the configuration of the CAMAC crate. When the control system is restarted it determines the configuration of the CAMAC crate from the `bl_define.def` file. The `bl_define.def` file for 8-1 follows:

```
#-----------------------------------------------------------------------------#
#                                                                             #
#  Device Definition File for: Beamline 8-1                                   #
#                                                                             #
#  Created by: userid                                                         #
#          On: time_date_stamp                                                #
#                                                                             #
#  More miscellaneous Comments etc.                                           #
#                                                                             #
#  The system uses the following as basic definitions for a given devices.   #
#  Having successfully read this file, it looks for definition files for     #
#  devices, such as motors, which need them.                                  #
#                                                                             #
#-----------------------------------------------------------------------------#
# Name          Type            Address Type:Number:Slot:Sub_address

hex$1           KS_3610         CAMAC:1:2:0
rtc$1           DSP_RTC_018     CAMAC:1:1:0
DAC             J_DA16          CAMAC:1:20:1

serp            PORT_1          SERIAL:1:0:0

GRATING         COMPU           serp:2:0:0
XSLIT           COMPU           serp:1:0:0

MONO            COMB
CMA             COMB
```

This listing contains the minimum devices required for the operation of the beam line.

The devices defined above are configured with device name, device type and address. The device name can be any descriptive name that is desired with the understanding that SUPER, XAS and the .prg codes may place requirements on the name of a particular device. For example SUPER will look for hex scalars with the name `hex$*` and a real time clock with the name `RTC$*`. Also the `mono.prg` code will look for motors with the names GRATING and XSLIT, and the cma.prg code looks for a motor named DAC.

The device type must match the physical device sitting at the address specified for that device name. If the device type does not match the device at the address the control program could crash. The device types for 8-1 and their corresponding real device are listed in Table 8

Device Type	Device Description
KS_3610	Kinetic Systems Hex Scalar #3610
DSP_RTC_018	DSP Real Time Clock
J_DA16	Joerger 16bit Digital to Analog Converter
PORT_1	Alpha Serial Port
COMPU	Compumotor SX Indexer/Drive
COMB	ICS combination Motor

Table 8 ICS Devices

The device address is simply given as bus_type:number:slot:sub_address. The bus types available to 8-1 are CAMAC and SERIAL. Since 8-1 only has one CAMAC crate the number for CAMAC devices is always one. Similarly since only port one is configured to work with the compumotor devices this number is also always one. Slot is the slot location of the device in the crate and sub_address is the address of the device in that particular module (E500 and J_DA16 have multiple devices per module). Note that the compumotors use a bus that is defined in the `bl_define.def` file as `serp`. This tells the control system that these devices are using the using the serial port and that commands should be sent using the compumotor syntax. Slot for these devices is the daisy-chain address as defined by a dip switch on the unit.

As the startup routine configures each device in the `bl_define.def` file it loads the parameters from the `.par` file and 'compiles' the associated `.prg` file if one is defined.

4.2 ICS_CONF

ICS_CONF will be the most frequently used ICS utility. This utility allows the user to move the motor to a position and define information about the motor such as scale, speed and software limits. To access the control panel type at the prompt:

```
81STEW>ics_conf grating
```

and Figure 30 will be displayed.

```
Device Name:       GRATING
Device Type:       COMPUMOTOR              Device Lock:  OFF
Device Status:     OK - ON LINE            Limits:       HIGH ON    LOW ON
Device Address:    SERP:2:0:0

Current Position:      -23330.000000     Current Steps:       -23330
Last Position:         -18595.000000     Last Steps:          -18595


Device Scale:          1.000000          Backlash Move:       -10
Scale Back:            1.000000          Direction:           FORWARDS
Device Units:          mm
Scaled Hi Lim:         10000000.000000   Unscaled Hi Lim:     10000000
Scaled Lo Lim:         -500000000.00000  Unscaled Lo Lim:     -500000000

Accel. time:           1.000000          Def. Accel. time:    1.000000
Slew Rate:             1.000000          Def. Slew Rate:      1.000000
Tolerance lim:         0
Poll Interval:         0.250000          Device Privilege:    DEFAULT

 MOVE      ABORT            RESET                HELP    PARAMS   EXIT
```

Figure 30 GRATING Motion Control Panel

The menu along the bottom of the control panel displays the commands that are available to the user. These commands are accessed by typing the first letter of the command. The commands are summarized in Table 9. To change a value tab or arrow to the position that you want to change and type return. Type in the number that you want and then type return again. You should be careful about hitting return in the control panel however because it is quite easy to change a value to zero.

Command	Description
Move	Moves the motor to a specified position.
Abort	Stops the motion of the motor immediately.
Reset	Performs a software reset of the motor.
Help	Displays the Help File.
Params	Moves to the parameter sub-panel.
Exit	Exits the control panel.

Table 9 ICS_CONF Commands

The three motors that are essential to 8-1 are GRATING, XSLIT and MONO. In order for the monochromator to work properly several parameters need to be defined in the PARAMS panel for the three devices.

4.2.1 ICS_CONF GRATING

Type `ics_conf grating` to view the control panel for the grating (Figure 30). Table 10 displays the key motion parameters for the grating.

Motion Parameter	Value
Scale	1

Accel. time	1
Slew Rate	1
Scaled Hi lim	3000
Scaled Lo lim	-60000

Table 10 GRATING Motion Parameters

Now type `p` to display the configuration parameters for the grating (Figure 31).

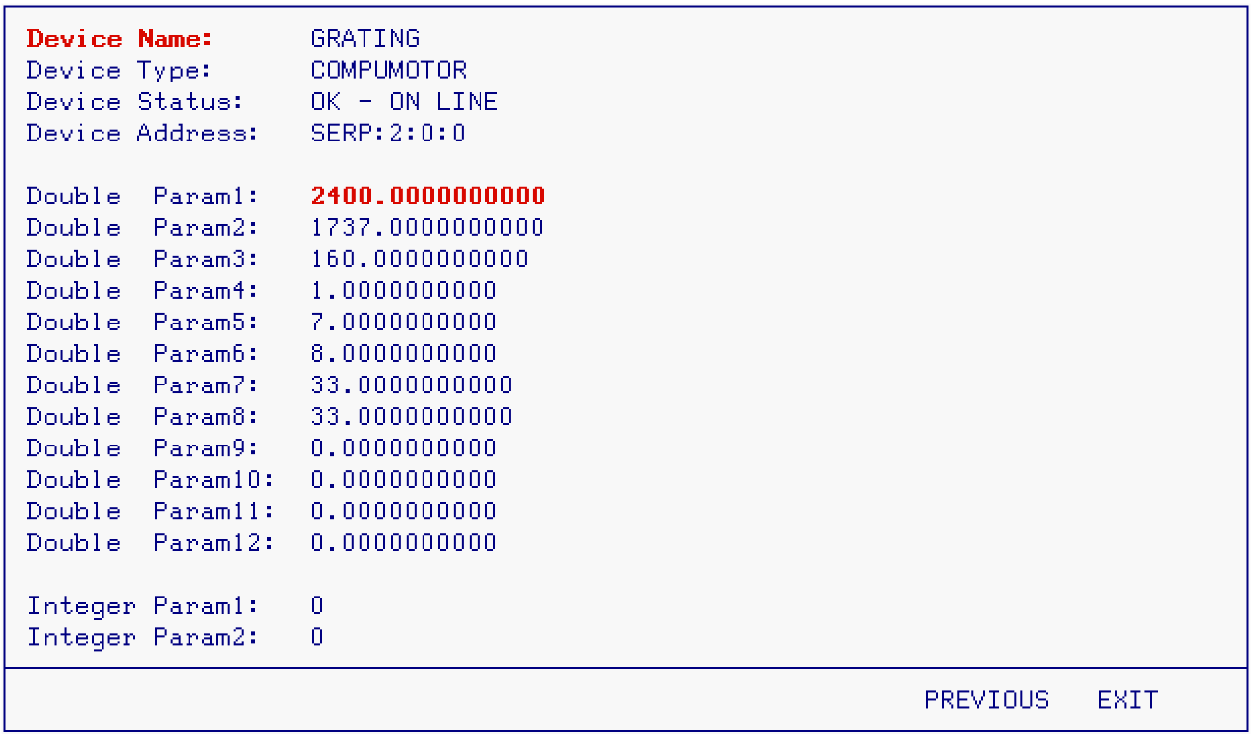

Figure 31 GRATING Configuration Parameters Control Panel

The configuration parameters for the grating are in Table 11.

Name	**Description**	**Nominal Values**
Double Param1	Lines per millimeter	288, 822, 2400 l/mm
Double Param2	Zero Order Position S_0'	Varies
Double Param3	Opening Angle	160°
Double Param4	Order	1, 2, 3 etc.
Double Param5	Energy 1 under old calibration E_1	Varies
Double Param6	Energy 1 under new calibration E_1'	Varies
Double Param7	Energy 2 under old calibration E_2	Varies
Double Param8	Energy 2 under new calibration E_2'	Varies

Table 11 GRATING Configuration Parameters

4.2.2 ICS_CONF XSLIT

Type `ics_conf xslit` at the prompt to view the motion control panel for the exit slit (Figure 32).

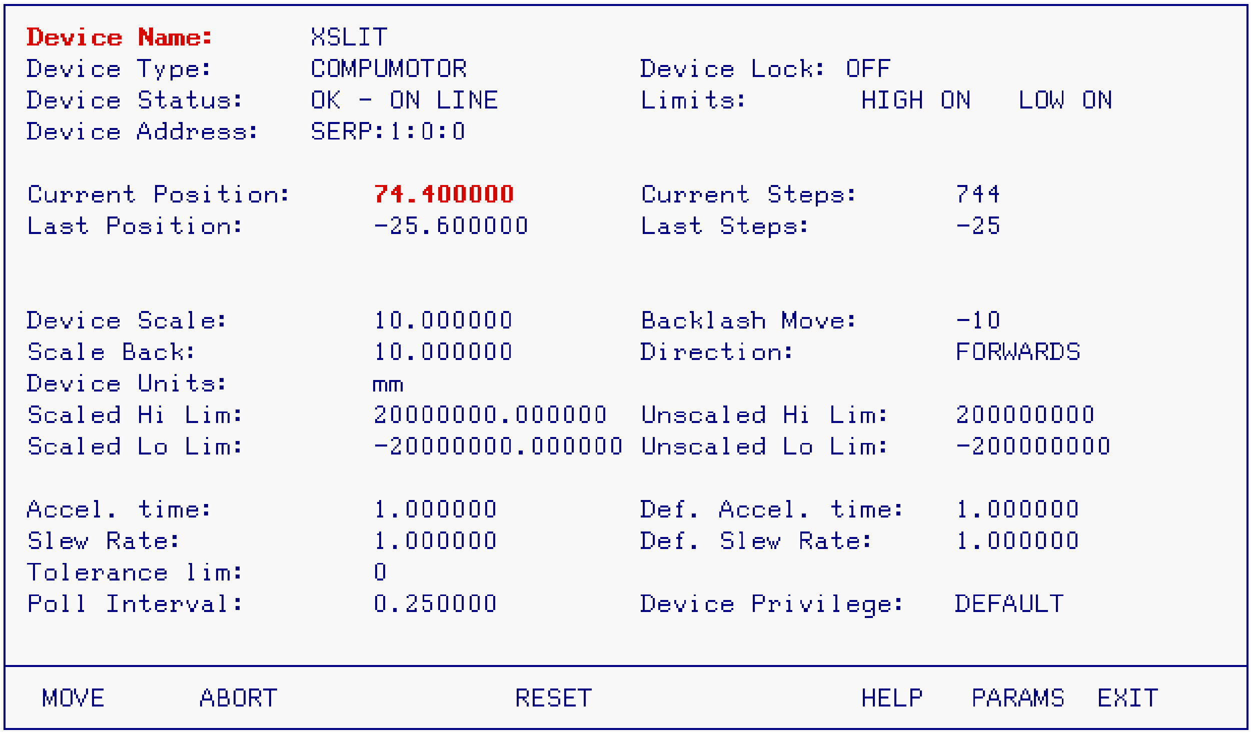

Figure 32 XSLIT Motion Control Panel

Table 12 displays the key motion parameters for the xslit.

Motion Parameter	Value
Scale	10
Accel. time	1
Slew Rate	1
Scaled Hi lim	
Scaled Lo lim	

Table 12 XSLIT Motion Parameters

Now type `p` in the motion control panel to display the configuration control panel (Figure 33). The configuration parameters for the XSLIT are given in Table 13.

Name	Description	Nominal Values
Double Param1	Saggital Radius of Curvature	19224 mm
Double Param2	Entrance Slit to grating distance	2100 mm

Table 13 XSLIT Configuration Parameters

```
Device Name:        XSLIT
Device Type:        COMPUMOTOR
Device Status:      OK - ON LINE
Device Address:     SERP:1:0:0

Double  Param1:     19224.0000000000
Double  Param2:     2111.0000000000
Double  Param3:     0.0000000000
Double  Param4:     0.0000000000
Double  Param5:     0.0000000000
Double  Param6:     0.0000000000
Double  Param7:     0.0000000000
Double  Param8:     0.0000000000
Double  Param9:     0.0000000000
Double  Param10:    0.0000000000
Double  Param11:    0.0000000000
Double  Param12:    0.0000000000

Integer Param1:     0
Integer Param2:     0

                                                                PREVIOUS   EXIT
```

Figure 33 XSLIT Configuration Control Panel

4.2.3 ICS_CONF MONO

The monochromator control panel is displayed with `ics_conf mono` (Figure 34).

```
Device Name:        MONO
Device Type:        COMB                    Device Lock:  OFF
Device Status:      OK - ON LINE            Limits:       HIGH OFF   LOW OFF
Device Address:     COMB:0:0:0


Current Position:       129.998278
Last Position:          160.002363


                                            Abort Correct:      YES
Device Units:           eV
Scaled Hi Lim:          200.000000
Scaled Lo Lim:          8.000000



Tracking:               0.000000
                                            Device Privilege:   DEFAULT

 MOVE      ABORT     CORRECT     RESET                  HELP    PARAMS   EXIT
```

Figure 34 MONO Motion Control Panel

Since MONO is a combination motor there are only parameters for the lower and upper limits and these are 8 and 200 eV respectively. Type `p` to display the configuration parameters (Figure 35).

```
Device Name:       MONO
Device Type:       COMB
Device Status:     OK - ON LINE
Device Address:    COMB:0:0:0

Double  Param1:    1737.0000000000  d-spacing
Double  Param2:    -5060.4664551670 channel width
Double  Param3:    -318.8159335166  asymmetric cut
Double  Param4:    1700.0000000000
Double  Param5:    -6554.3825770000
Double  Param6:    -15.2919105000
Double  Param7:    1769.0000000000
Double  Param8:    -6601.1986110000
Double  Param9:    -10.7162483200
Double  Param10:   1.0000000000
Double  Param11:   0.0000000000
Double  Param12:   0.0000000000

Integer Param1:    0
Integer Param2:    0

                                                PREVIOUS   EXIT
```

Figure 35 MONO Configuration Parameters

The configuration parameters are given in Table 14.

Name	Description	Nominal Values
Double Param1	288 Calibration Coefficient C_0	Varies, equals ZOP
Double Param2	288 Calibration Coefficient C_1	Varies
Double Param3	288 Calibration Coefficient C_2	Varies
Double Param4	822 Calibration Coefficient C_0	Varies, equals ZOP
Double Param5	822 Calibration Coefficient C_1	Varies
Double Param6	822 Calibration Coefficient C_2	Varies
Double Param7	2400 Calibration Coefficient C_0	Varies, equals ZOP
Double Param8	2400 Calibration Coefficient C_1	Varies
Double Param9	2400 Calibration Coefficient C_2	Varies
Double Param10	Geometrical Transfer / Calibrated Transfer	0 / 1
Double Param11	Normal Operation / Calibrate Mono	0 / 1
Double Param12	Fixed Exit Slit / Move Exit Slit	0 / 1

Table 14 MONO Configuration Parameters

4.2.3.1 Calibrating the Monochromator

The last three parameters for MONO are switches that affect the way the software operates. Double Param10 (DP10) determines whether the geometrical or calibrated transfer equations are used to calculate the energy of the mono. The switch DP11 when set to 1 tells the mono to calculate new coefficients using the method in 2.4.8, with S_0', E_1, E_1', E_2, E_2', from grating configuration parameters DP2, DP5, DP6, DP7 and DP8 respectively. After the new coefficients are calculated mono configuration DP11 is reset to 0.

5. Beam Line Checkout

5.1 Intent

The intent behind performing the beam line checkout is to ensure that when a user goes on line the beam line is operating as advertised, and to record the performance of the beam line over an extended period of time. Both reasons allow us to identify faults with the beam line from the immediate such as miss-calibrated slits or broken electronics to the long term such as degradation of the optical elements due to contamination.

The checkout procedure is a straightforward set of measurements that covers zero order as well as the entire energy range of the gratings. These measurements are collected as a series of scans as detailed on the checkout sheet. In addition measurements are taken at various slit settings and energies.

The scans allow us to look for regular features in the transmission functions of the gratings. If the intensity of these features differs significantly we know to look for possible alignment or aperturing problems. If these features are expanded or contracted we should look for mechanical problems such as a failing encoder or stepper motor, or typos in the parameters for that particular grating. If the scans are noisy we should check that our data acquisition electronics are in good working order.

The measurements at various energies and slit settings allows us to again determine if there are aperturing problems with the beam line. Above all these measurements when taken in aggregate show us whether there is long term degradation of the beam line due to contamination.

5.2 Set Up

At this time all of the data collected should be done using the photo diode just upstream of the refocussing mirror. After we have installed an evaporator for the I_0 grid all measurements will be collected after the refocussing mirror. The checkout sheet contains lots of useful information and during the course of the checkout it will be handy to have the last checkout sheet available (section 5.4). Position the diode and set the entrance and exit slits to 100 x 100 µm.

Connect the signal line of the diode to a Keithley 427 amplifier and connect the bias line of the diode to a Fluke 415b power supply and set the bias voltage to 100 V. Connect one output of the Keithley to a DVM and the other to a voltage to frequency converter. The polarity of the v-f converter should be negative. Connect the output of the v-f converter to one of the hex scalar channels in the CAMAC crate. A useful test at this point is to set the suppression to match the gain of the Keithley and adjust the suppression knob until the DVM reads some negative number. Use the computer to count for 1 second and verify that the collected data and the DVM reading have some resemblance to each other (nominally the relationship should be 100,000 counts per volt, but this will depend on the v-f settings). After verifying that the data acquisition chain works return the suppression to off and begin the checkout.

5.3 Procedure

With the diode in place move grating to it's zero order position as recorded on the previous checkout sheet. Set the gain of the Keithley to the previous setting and then adjust the vertical tilt of the M0 mirror to maximize the reading from the Keithley. Scan the grating using the parameters given on the checkout sheet and fill in the appropriate values.

After recording the zero order spectra, move the monochromator to an appropriate energy (this is given as the Flux at xxx eV blank on the checkout sheet) and again adjust the vertical tilt of the M0 mirror for maximum intensity with the Keithley set to the appropriate gain. Now scan the monochromator using the parameters on the checkout sheet and again fill in the requested information.

Finally move the monochromator to the three requested energies, adjusting the M0 tilt at each point and record the intensity (both voltage and gain). Repeat this for 50 x 50 µm.

Repeat this for the remaining gratings and the checkout is complete.

5.4 Checkout Sheet

8-1 Checkout Sheet

Mono Zero Position OK:_______ Mono Motion OK:_________
Slit Zero Positions OK:________ Slit Motion OK:_____ _____

Down Stream Photodiode, Entrance Slit and Exit slit at 100µ 100V bias voltage

288 l/mm Grating Zero order scan.
-500 – +200 steps, 10 steps/interval, 1s/point
File Name:___________DCCT:_____Kiethley Gain:_____Peak DVM Voltage:_____
Maximum Flux@:______________motor steps

288 l/mm Grating Energy scan.
8 - 35 eV, 1 eV/interval, 1s/point
File Name:___________DCCT:___Kiethley Gain:_________Flux at 20eV:_________

Energy	Flux at 100x100µ	Flux at 50x50µ
10eV		
19eV		
33eV		
DCCT		

822 l/mm Grating Zero order scan.
-500 – +200 steps, 10 steps/interval, 1s/point
File Name:___________DCCT:_____Kiethley Gain:_____Peak DVM Voltage:_____
Maximum Flux@:______________motor steps

822 l/mm Grating Energy scan.
20 - 120 eV, 1 eV/interval, 1s/point
File Name:___________DCCT:___Kiethley Gain:_________Flux at 80eV:_________

Energy	Flux at 100x100µ	Flux at 50x50µ
25eV		
70eV		
105eV		
DCCT		

2400 l/mm Grating Zero order scan.
-500 – +200 steps, 10 steps/interval, 1s/point
File Name:___________DCCT:_____Kiethley Gain:_____Peak DVM Voltage:_____
Maximum Flux@:______________motor steps

2400 l/mm Grating Energy scan.
60 - 200 eV, 1 eV/interval, 1s/point
File Name:___________DCCT:___Kiethley Gain:_________Flux at 120eV:________

Energy	Flux at 100x100µ	Flux at 50x50µ
65eV		
130eV		
190eV		
DCCT		

Max Flux on M0 mirror:(m1)_______ (m2)________ (m3)_________ (m4)_________

Notes:

Appendix 1 The Optical Path Function

The Vertex Equation

The optical path function is defined as the distance a ray of light would travel through an optical system from source to image point. Our optical system consists of a toroidal grating whose axis of revolution is defined in (Figure 36). From the coordinate system of Figure 36 we have for the equation of a toroid:

$$\left[\left(x'^2 + y'^2\right)^{1/2} - (R-\rho)\right]^2 + z'^2 = \rho^2$$

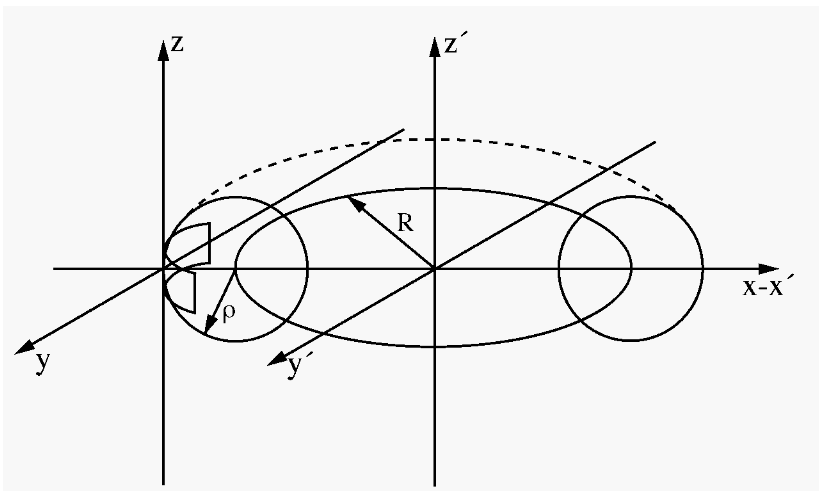

Figure 36 Toroidal Grating Nomenclature

We want to use the coordinate transform equations

$$x' = x - R; \quad y' = y; \quad z' = z$$

to move the system to the unprimed coordinates.

If we let

$$x'^2 + y'^2 = L^2$$

we can derive a vertex equation for the toroid:

$$\left[L - (R-\rho)\right]^2 + z'^2 = \rho^2$$

$$L^2 - 2L(R-\rho) + (R-\rho)^2 + z'^2 = \rho^2$$

$$x'^2 + y'^2 + z'^2 = \rho^2 + 2L(R-\rho) - (R-\rho)^2$$

and with the application of the transform equations:

$$(x-R)^2+y^2+z^2=\rho^2+2\left[(x-R)^2+y^2\right]^{1/2}(R-\rho)-(R-\rho)^2$$

$$x^2-2Rx+R^2+y^2+z^2=\rho^2+2\left[(x-R)^2+y^2\right]^{1/2}(R-\rho)-(R-\rho)^2$$

and our vertex equation becomes

$$x^2+y^2+z^2=2Rx+2\left[(x-R)^2+y^2\right]^{1/2}(R-\rho)+\left[\rho^2-(R-\rho)^2-R^2\right]$$

reducing the rightmost term in square brackets yields

$$x^2+y^2+z^2=2Rx-2\left[(x-R)^2+y^2\right]^{1/2}(R-\rho)-2R(R-\rho)$$

and if we let

$$(x-R)^2=(R-x)^2=J^2$$

we have

$$x^2+y^2+z^2=2Rx-2R(R-\rho)+2\left(J^2+y^2\right)^{1/2}(R-\rho)$$

$$=2Rx-2R(R-\rho)+2(R-\rho)J\left(1+\frac{y^2}{J^2}\right)^{1/2}$$

and using the case J = (R - x)

$$=2Rx-2R(R-\rho)+2(R-\rho)(R-x)\left(1+\frac{y^2}{(R-x)^2}\right)^{1/2}.$$

In order to provide a solution that is expressed as a function of x, y, and z with no terms in the denominator, we will use a number of power series expansions, of which the generalized form is:

$$(S\pm T)^n=S^n\pm nS^{n-1}T+\frac{n(n-1)S^{n-2}T^2}{2!}\pm\frac{n(n-1)(n-2)S^{n-3}T^3}{3!}+\frac{n(n-1)(n-2)(n-3)S^{n-4}T^4}{4!}\pm\ldots$$

By making the proper selection of S, T and n we can make all of the expansions necessary for our path function. At this point it is also useful to set the limits of the expansion to the sixth order in y.

In order to expand our term under the square root our power series expansion becomes

$$(1+T)^{1/2} = 1 + \frac{T}{2} - \frac{T^2}{8} + \frac{T^3}{16} - \dots$$

where S = 1 and n =1/2 and we have

$$\left(1+\frac{y^2}{(R-x)^2}\right)^{1/2} = 1 + \frac{y^2}{2(R-x)^2} - \frac{y^4}{8(R-x)^4} + \frac{y^6}{16(R-x)^6} - \dots$$

Factoring out the 1 allows us to simplify the terms without any y dependence:

$$2Rx - 2R(R-\rho) + 2(R-\rho)(R-x) = 2Rx - 2Rx - 2R^2 + 2R^2 + 2R\rho - 2R\rho - 2\rho x = 2\rho x$$

and our vertex equation is now

$$x^2 + y^2 + z^2 = 2\rho x + 2(R-\rho)(R-x)\left[\frac{y^2}{2(R-x)^2} - \frac{y^4}{8(R-x)^4} + \frac{y^6}{16(R-x)^6} - \dots\right].$$

Next we want to expand the terms in square brackets to remove x from the denominator. First we make the following simplification:

$$\frac{y^2}{2(R-x)^2} = \frac{y^2}{2R^2\left(1-\frac{x}{R}\right)^2} = \frac{y^2}{2R^2}\left(\frac{1}{(1-T)^2}\right)$$

where

$$T = \frac{x}{R}.$$

Our power series expansion then becomes

$$(1-T)^{-2} = 1 + 2T + 3T^2 + 4T^3 + \dots$$

and applying this out to the second order in x we get

$$\frac{y^2}{2(R-x)^2} = \frac{y^2}{2R^2}\left[1 + \frac{2x}{R} + \frac{3x^2}{R^2}\right]$$

$$\frac{y^4}{8(R-x)^4} = \frac{y^4}{8R^4}\left[1 + \frac{4x}{R} + \frac{10x^2}{R^2}\right]$$

$$\frac{y^6}{16(R-x)^6} = \frac{y^6}{16R^6}\left[1 + \frac{6x}{R} + \frac{21x^2}{R^2}\right]$$

and our vertex equation is

$$x^2 + y^2 + z^2 = 2\rho x + \left(2R(R-\rho) - 2x(R-\rho)\right) \bullet$$
$$\left[\frac{y^2}{2R^2}\left[1 + \frac{2x}{R} + \frac{3x^2}{R^2}\right] + \frac{y^4}{8R^4}\left[1 + \frac{4x}{R} + \frac{10x^2}{R^2}\right] + -\frac{y^6}{16R^6}\left[1 + \frac{6x}{R} + \frac{21x^2}{R^2}\right]\right]$$

If we define

$$\Omega = \left(1 - \frac{\rho}{R}\right)$$

we have

$$2(R-\rho)(R-x) = 2R^2\Omega\left(1 - \frac{x}{R}\right)$$

and after multiplying through and simplifying we have

$$x^2 + y^2 + z^2 = 2\rho x + y^2[\Omega] + xy^2\left[\frac{\Omega}{R}\right] + x^2y^2\left[\frac{\Omega}{R^2}\right] + y^4\left[-\frac{\Omega}{4R^2}\right]$$
$$+ xy^4\left[-\frac{3\Omega}{4R^3}\right] + x^2y^4\left[-\frac{3\Omega}{2R^4}\right] + y^6\left[\frac{\Omega}{8R^4}\right] + xy^6\left[\frac{5\Omega}{8R^5}\right] + x^2y^6\left[\frac{15\Omega}{8R^6}\right]$$

Rowland Gratings

If we define our source point to be at A with coordinates (x_a,y_a,z_a), our image point to be at B with coordinates (x_b,y_b,z_b), and let the point P lie on the surface of the grating with coordinates (x,y,z) where P is limited to discrete values of y due to the presence of a grating (y is at some groove n), we can define the path length function as (Figure 37):

$$F = \langle AP \rangle + \langle PB \rangle + m\lambda n = \langle AP \rangle + \langle PB \rangle + \frac{m\lambda y}{d}.$$

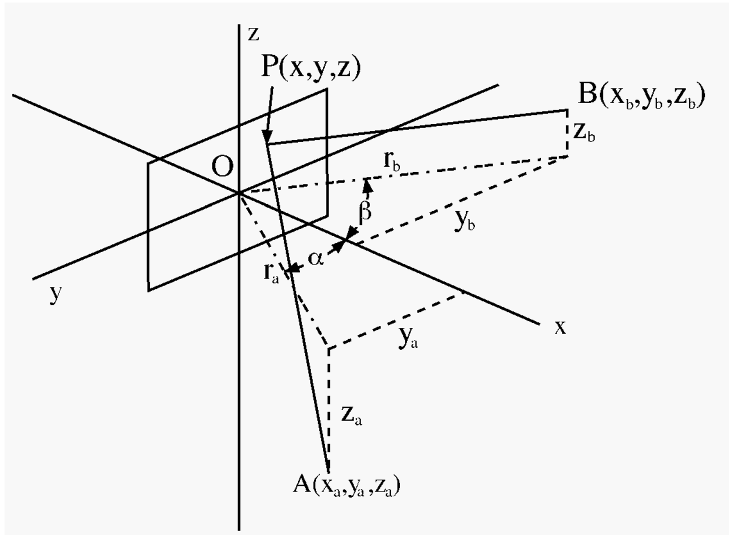

Figure 37 Path Length Function Coordinate System

Now the square of the distance from A to P is

$$\langle AP\rangle^2 = (x - x_a)^2 + (y - y_a)^2 + (z - z_a)^2$$

expanding this we have

$$= x^2 - 2xx_a + x_a{}^2 + y^2 - 2yy_a + y_a{}^2 + z^2 - 2zz_a + z_a{}^2$$

$$= x_a{}^2 + y_a{}^2 + z_a{}^2 - 2xx_a - 2yy_a - 2zz_a + x^2 + y^2 + z^2.$$

If we define r_a as the distance from A to the origin in the xy plane we have

$$r_a{}^2 = x_a{}^2 + y_a{}^2$$

and

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 - 2xx_a - 2yy_a - 2zz_a + x^2 + y^2 + z^2.$$

Applying now our vertex equation we have

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 + 2x(\rho - x_a) - 2yy_a - 2zz_a + y^2[\Omega] + xy^2\left[\frac{\Omega}{R}\right] + x^2y^2\left[\frac{\Omega}{R^2}\right] + y^4\left[-\frac{\Omega}{4R^2}\right]$$
$$+ xy^4\left[-\frac{3\Omega}{4R^3}\right] + x^2y^4\left[-\frac{3\Omega}{2R^4}\right] + y^6\left[\frac{\Omega}{8R^4}\right] + xy^6\left[\frac{5\Omega}{8R^5}\right] + x^2y^6\left[\frac{15\Omega}{8R^6}\right]$$

If we solve for 2x from the vertex equation we have

$$2x = \frac{1}{\rho}\left\{\begin{matrix} x^2 + y^2 + z^2 - y^2[\Omega] - xy^2\left[\frac{\Omega}{R}\right] - x^2y^2\left[\frac{\Omega}{R^2}\right] + y^4\left[\frac{\Omega}{4R^2}\right] \\ + xy^4\left[\frac{3\Omega}{4R^3}\right] + x^2y^4\left[\frac{3\Omega}{2R^4}\right] - y^6\left[\frac{\Omega}{8R^4}\right] - xy^6\left[\frac{5\Omega}{8R^5}\right] - x^2y^6\left[\frac{15\Omega}{8R^6}\right] \end{matrix}\right\}$$

and now

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 + \left(1 - \frac{x_a}{\rho}\right)\left\{\begin{matrix} x^2 + y^2 + z^2 - y^2[\Omega] - xy^2\left[\frac{\Omega}{R}\right] - x^2y^2\left[\frac{\Omega}{R^2}\right] + y^4\left[\frac{\Omega}{4R^2}\right] \\ + xy^4\left[\frac{3\Omega}{4R^3}\right] + x^2y^4\left[\frac{3\Omega}{2R^4}\right] - y^6\left[\frac{\Omega}{8R^4}\right] - xy^6\left[\frac{5\Omega}{8R^5}\right] - x^2y^6\left[\frac{15\Omega}{8R^6}\right] \end{matrix}\right\}$$
$$+ y^2[\Omega] + xy^2\left[\frac{\Omega}{R}\right] + x^2y^2\left[\frac{\Omega}{R^2}\right] + y^4\left[-\frac{\Omega}{4R^2}\right] + xy^4\left[-\frac{3\Omega}{4R^3}\right] + x^2y^4\left[-\frac{3\Omega}{2R^4}\right] + y^6\left[\frac{\Omega}{8R^4}\right]$$
$$+ xy^6\left[\frac{5\Omega}{8R^5}\right] + x^2y^6\left[\frac{15\Omega}{8R^6}\right] - 2yy_a - 2zz_a$$

If we define

$$\omega = \left(1 - \frac{x_a}{\rho}\right)$$

we have after simplification and combination of like terms

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 + \omega x^2 + \omega z^2 + y^2\left[1 - \frac{x_a}{R}\right] + xy^2\left[\frac{\Omega x_a}{R\rho}\right] + x^2y^2\left[\frac{\Omega x_a}{R^2\rho}\right] + y^4\left[-\frac{\Omega x_a}{4R^2\rho}\right]$$
$$+ xy^4\left[-\frac{3\Omega x_a}{4R^3\rho}\right] + x^2y^4\left[-\frac{3\Omega x_a}{2R^4\rho}\right] + y^6\left[\frac{\Omega x_a}{8R^4\rho}\right] + xy^6\left[\frac{5\Omega x_a}{8R^5\rho}\right] + x^2y^6\left[\frac{15\Omega x_a}{8R^6\rho}\right]$$
$$-2yy_a - 2zz_a$$

At this point it would be useful to eliminate x and x^2. Using the vertex equation and making the following substitutions

$$A = \frac{\Omega}{R}\ ;\ B = \frac{\Omega}{R^2}\ ;\ C = -\frac{\Omega}{4R^2}\ ;\ D = -\frac{3\Omega}{4R^3};$$

and

$$E = -\frac{3\Omega}{2R^4}\ ;\ F = \frac{\Omega}{8R^4}\ ;\ G = \frac{5\Omega}{8R^5}\ ;\ H = \frac{15\Omega}{8R^6}$$

we can reduce our vertex equation to a quadratic equation

$$x^2\left(1 - By^2 - Ey^4 - Hy^6\right) + x\left(-2\rho - Ay^2 - Dy^4 - Gy^6\right) + \left(y^2 + z^2 - \Omega y^2 - Cy^4 - Fy^6\right) = 0.$$

Using the quadratic equation we can solve for x

$$x=\frac{-b\pm\sqrt{b^2-4ac}}{2a}.$$

If we examine our path function we see that x is always multiplied by y^2 at the minimum. Since we are keeping only those terms of sixth order or less we can eliminate those terms in the solution for x which are greater than fourth order. Now calculating the terms we have

$$-b=2\rho+Ay^2+Dy^4+Gy^6$$

$$b^2=4\rho^2+4\rho Ay^2+4\rho Dy^4+4\rho Gy^6+A^2y^4+2ADy^6$$

$$-4ac=-4y^2-4z^2+4\Omega y^2+4Cy^4+4Fy^6+4By^4+4By^2z^2$$
$$-4B\Omega y^4-4BCy^6+4Ey^6+4Ey^4z^2-4E\Omega y^6$$

and

$$b^2-4ac=4\rho^2+y^2\left(-\frac{4\rho^2}{R^2}\right)-4z^2+y^2z^2\left(\frac{4\Omega}{R^2}\right)+y^4z^2\left(-\frac{6\Omega}{R^4}\right)+y^6\left(-\frac{3\rho\Omega}{R^5}\right)$$

We can take the square root with the expansion

$$(S+T)^{1/2}=S^{1/2}+\frac{T}{2S^{1/2}}-\frac{T^2}{8S^{3/2}}+\frac{T^3}{16S^{5/2}}\ldots$$

where

$$S=4\rho^2$$

and T is the remainder. This yields

$$\sqrt{b^2-4ac}=2\rho+y^2\left(-\frac{\rho}{R^2}\right)+z^2\left(-\frac{1}{\rho}\right)+y^2z^2\left(\frac{\Omega}{R^2\rho}-\frac{1}{2R^2\rho}\right)+y^4\left(-\frac{\rho}{4R^4}\right)$$
$$+z^4\left(\frac{1}{4\rho^3}\right)+y^2z^4\left(\frac{\Omega}{2R^2\rho^3}-\frac{1}{4R^2\rho^3}\right)+y^4z^2\left(\frac{\Omega}{2R^4\rho}-\frac{1}{4R^4\rho}\right)+y^6\left(-\frac{3\Omega}{4R^5}-\frac{\rho}{8R^6}\right)$$

and taking the negative root yields

$$-b-\sqrt{b^2-4ac}=y^2\left(\frac{1}{R}\right)+z^2\left(\frac{1}{\rho}\right)+y^2z^2\left(\frac{1}{2R^2\rho}-\frac{\Omega}{R^2\rho}\right)+y^4\left(\frac{\rho}{4R^4}-\frac{3\Omega}{4R^3}\right)+z^4\left(\frac{1}{4\rho^3}\right)$$
$$+y^2z^4\left(\frac{1}{4R^2\rho^3}-\frac{\Omega}{2R^2\rho^3}\right)+y^4z^2\left(\frac{1}{4R^4\rho}-\frac{\Omega}{2R^4\rho}\right)+y^6\left(\frac{11\Omega}{8R^5}-\frac{\rho}{8R^6}\right)$$

Expanding the denominator 2a in the form

$$\frac{1}{1+T} = 1 - T + T^2 - T^3 + \ldots$$

yields

$$\frac{1}{2a} = \frac{1}{2}\left(\frac{1}{1 - By^2 - Ey^4 - Hy^6}\right) = \frac{1}{2}\left(1 + By^2 + Ey^4 + Hy^6 + 2BEy^6 - B^3y^6\right).$$

After multiplying and collecting terms we have

$$x = \frac{y^2}{2R} + \frac{z^2}{2\rho} + \frac{y^2z^2}{4R^2\rho} + \frac{y^4}{8R^3} + \frac{z^4}{8\rho^3}$$

and

$$x^2 = \frac{y^4}{4R^2} + \frac{z^4}{4\rho^2} + \frac{y^2z^2}{2R\rho} + y^2z^4\left(\frac{1}{8R\rho^3} + \frac{1}{4R^2\rho^2}\right) + y^4z^2\left(\frac{3}{8R^3\rho}\right) + \frac{y^6}{8R^4}.$$

Inserting x and x^2 into our path function and multiplying and sorting terms yields

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 - 2zz_a - 2yy_a + y^2\left(1 - \frac{x_a}{R}\right) + z^2\left(1 - \frac{x_a}{\rho}\right) + \frac{y^2z^2}{2R\rho}\left(1 - \frac{x_a}{R}\right) + \frac{y^4}{4R^2}\left(1 - \frac{x_a}{R}\right)$$
$$+ \frac{z^4}{4\rho^2}\left(1 - \frac{x_a}{\rho}\right) + y^2z^4\left(\frac{1}{8R\rho^3}\left(1 - \frac{x_a}{R}\right) + \frac{1}{4R^2\rho^2}\left(1 - \frac{x_a}{R}\right)\right) + y^4z^2\left(\frac{3}{8R^3\rho} - \frac{3x_a}{8R^4\rho}\right) + \frac{y^6}{8R^4}\left(1 - \frac{x_a}{R}\right)$$

From Figure 37 our coordinate system allows us to make a transformation to cylindrical coordinates with the following formulae

$$x_a = r_a\cos\alpha\ ;\ y_a = r_a\sin\alpha.$$

This transform gives us

$$\langle AP\rangle^2 = r_a{}^2 + z_a{}^2 - 2zz_a - 2yr_a\sin\alpha + y^2\left(1 - \frac{r_a\cos\alpha}{R}\right) + z^2\left(1 - \frac{r_a\cos\alpha}{\rho}\right) + \frac{y^2z^2}{2R\rho}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$
$$+ \frac{y^4}{4R^2}\left(1 - \frac{r_a\cos\alpha}{R}\right) + \frac{z^4}{4\rho^2}\left(1 - \frac{r_a\cos\alpha}{\rho}\right) + y^2z^4\left(\frac{1}{8R\rho^3}\left(1 - \frac{r_a\cos\alpha}{R}\right) + \frac{1}{4R^2\rho^2}\left(1 - \frac{r_a\cos\alpha}{R}\right)\right)$$
$$+ y^4z^2\left(\frac{3}{8R^3\rho} - \frac{3r_a\cos\alpha}{8R^4\rho}\right) + \frac{y^6}{8R^4}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$

and if we expand the y^2 term and use the identity $y^2 = y^2\sin^2\alpha + y^2\cos^2\alpha$ to borrow a $y^2\sin^2\alpha$ term, and then recombine that with $r_a{}^2$ and $-2yr_a\sin\alpha$ we have

$$\langle AP\rangle^2 = (r_a - y\sin\alpha)^2 + y^2\left(\cos^2\alpha - \frac{r_a\cos\alpha}{R}\right) + z^2\left(1 - \frac{r_a\cos\alpha}{\rho}\right) + \frac{y^2z^2}{2R\rho}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$
$$+\frac{y^4}{4R^2}\left(1 - \frac{r_a\cos\alpha}{R}\right) + \frac{z^4}{4\rho^2}\left(1 - \frac{r_a\cos\alpha}{\rho}\right) + y^2z^4\left(\frac{1}{8R\rho^3}\left(1 - \frac{r_a\cos\alpha}{R}\right) + \frac{1}{4R^2\rho^2}\left(1 - \frac{r_a\cos\alpha}{R}\right)\right)$$
$$+y^4z^2\left(\frac{3}{8R^3\rho} - \frac{3r_a\cos\alpha}{8R^4\rho}\right) + \frac{y^6}{8R^4}\left(1 - \frac{r_a\cos\alpha}{R}\right) + z_a{}^2 - 2zz_a$$

Now we need to take the square root of the above function using the expansion

$$(S+T)^{1/2} = S^{1/2} + \frac{T}{2S^{1/2}} - \frac{T^2}{8S^{3/2}} + \frac{T^3}{16S^{5/2}} - \ldots$$

where we let

$$S = (r_a - y\sin\alpha)^2$$

and T is the remainder. If we make the following substitutions

$$A = \cos^2\alpha - \frac{r_a\cos\alpha}{R} \;;\; B = 1 - \frac{r_a\cos\alpha}{\rho}$$

$$C = \frac{1}{2R\rho}\left(1 - \frac{r_a\cos\alpha}{R}\right) \;;\; D = \frac{1}{4R^2}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$

$$E = \frac{1}{4\rho^2}\left(1 - \frac{r_a\cos\alpha}{\rho}\right) \;;\; F = \frac{1}{8R\rho^3}\left(1 - \frac{r_a\cos\alpha}{R}\right) + \frac{1}{4R^2\rho^2}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$

$$G = \frac{3}{8R^3\rho}\left(1 - \frac{r_a\cos\alpha}{R}\right) \quad H = \frac{1}{8R^4}\left(1 - \frac{r_a\cos\alpha}{R}\right)$$

and

$$J = z_a{}^2 - 2zz_a$$

we have

$$T = Ay^2 + Bz^2 + Cz^2y^2 + Dy^4 + Ez^4 + Fy^2z^4 + Gy^4z^2 + Hy^6 + J$$

$$T^2 = A^2y^4 + B^2z^4 + J^2 + 2ABy^2z^2 + 2(AE + BC)y^2z^4 + 2(AC + BD)y^4z^2$$
$$+2ADy^6 + 2AJy^2 + 2BJz^2 + 2CJy^2z^2 + 2DJy^4 + 2EJz^4$$

and

$$T^3 = A^3y^6 + 3AB^2y^2z^4 + 3AJ^2y^2 + 3A^2By^4z^2 + 3A^2Jy^4 + 6ABJy^2z^2 + 3BJ^2z^2 + 3B^2Jz^4$$

and our expansion yields

$$\langle AP \rangle = r_a - y\sin\alpha + \frac{T}{2(r_a - y\sin\alpha)} - \frac{T^2}{8(r_a - y\sin\alpha)^3} + \frac{T^3}{16(r_a - y\sin\alpha)^5}.$$

Expanding now our denominators we have

$$\frac{1}{2(r_a - y\sin\alpha)} = \frac{1}{2}\left\{\frac{1}{r_a} + \frac{y\sin\alpha}{r_a^{\ 2}} + \frac{y^2\sin^2\alpha}{r_a^{\ 3}} + \frac{y^3\sin^3\alpha}{r_a^{\ 4}} + \frac{y^4\sin^4\alpha}{r_a^{\ 5}}\right\}$$

$$\frac{1}{8(r_a - y\sin\alpha)^3} = \frac{1}{8}\left\{\frac{1}{r_a^{\ 3}} + \frac{3y\sin\alpha}{r_a^{\ 4}} + \frac{6y^2\sin^2\alpha}{r_a^{\ 5}} + \frac{10y^3\sin^3\alpha}{r_a^{\ 6}} + \frac{15y^4\sin^4\alpha}{r_a^{\ 7}}\right\}$$

and

$$\frac{1}{16(r_a - y\sin\alpha)^5} = \frac{1}{16}\left\{\frac{1}{r_a^{\ 5}} + \frac{5y\sin\alpha}{r_a^{\ 6}} + \frac{15y^2\sin^2\alpha}{r_a^{\ 7}} + \frac{35y^3\sin^3\alpha}{r_a^{\ 8}} + \frac{70y^4\sin^4\alpha}{r_a^{\ 9}}\right\}$$

At this point it is useful to determine which factors we want to keep. If we adopt the notation

$$AP_{ijk} \Leftrightarrow AP\left(y^i, z^j, z_a^k\right)$$

we can define the terms we want to keep with the following rules:

$$\begin{aligned} i &\le 6 \\ j &\le 4 \\ k &\le 2 \\ i + j + k &\le 6 \\ j + k &= \text{even} \end{aligned}$$

Given these rules, and after multiplying and sorting like terms in y and z and z_a we have

$$\begin{aligned} \langle AP \rangle = r_a &+ AP_{100} + AP_{200} + AP_{300} + AP_{400} + AP_{500} + AP_{600} + AP_{020} + AP_{120} \\ &+ AP_{220} + AP_{320} + AP_{420} + AP_{040} + AP_{140} + AP_{240} + AP_{011} + AP_{111} + AP_{211} \\ &+ AP_{311} + AP_{411} + AP_{002} + AP_{102} + AP_{202} + AP_{302} + AP_{402} + AP_{031} + AP_{131} \\ &+ AP_{231} + AP_{042} + AP_{013} + AP_{022} + AP_{122} + AP_{222} \end{aligned}$$

The above process may now be repeated for the distance from P to B to yield an identical function with the substitutions

$$r_a \to r_b \text{ and } \alpha \to \beta$$

and we have

$$\begin{aligned}\langle PB\rangle = r_b &+ PB_{100} + PB_{200} + PB_{300} + PB_{400} + PB_{500} + PB_{600} + PB_{020} + PB_{120}\\ &+PB_{220} + PB_{320} + PB_{420} + PB_{040} + PB_{140} + PB_{240} + PB_{011} + PB_{111} + PB_{211}\\ &+PB_{311} + PB_{411} + PB_{002} + PB_{102} + PB_{202} + PB_{302} + PB_{402} + PB_{031} + PB_{131}\\ &+PB_{231} + PB_{042} + PB_{013} + PB_{022} + PB_{122} + PB_{222}\end{aligned}$$

If we define

$$F_{ijk} = AP_{ijk} + PB_{ijk}$$

with the exception

$$F_{100} = AP_{100} + PB_{100} + \frac{m\lambda y}{d}$$

we have for our path length function

$$\begin{aligned}\langle AP\rangle + \langle PB\rangle + \frac{m\lambda y}{d} = r_a + r_b &+ F_{100} + F_{200} + F_{300} + F_{400} + F_{500} + F_{600} + F_{020} + F_{120}\\ &+F_{220} + F_{320} + F_{420} + F_{040} + F_{140} + F_{240} + F_{011} + F_{111} + F_{211}\\ &+F_{311} + F_{411} + F_{002} + F_{102} + F_{202} + F_{302} + F_{402} + F_{031} + F_{131}\\ &+F_{231} + F_{042} + F_{013} + F_{022} + F_{122} + F_{222}\end{aligned}$$

where if we make the following abbreviations

$$S_{a/b} = \left(\frac{1}{r_{a/b}} - \frac{\cos\alpha/\beta}{\rho}\right); T_{a/b} = \left(\frac{\cos^2\alpha/\beta}{r_{a/b}} - \frac{\cos\alpha/\beta}{R}\right); \text{ and } U_{a/b} = \left(\frac{1}{r_{a/b}} - \frac{\cos\alpha/\beta}{R}\right)$$

we have the following:

$$F_{100} = y\left(\frac{m\lambda}{d} - \sin\alpha - \sin\beta\right); \text{ the grating equation}$$

$$F_{200} = y^2\left(\frac{T_a}{2} + \frac{T_b}{2}\right); \text{ defocus}$$

$$F_{300} = y^3\left(\frac{\sin\alpha}{2r_a}T_a + \frac{\sin\beta}{2r_b}T_b\right); \text{ coma}$$

$$F_{400}=y^4\left(\frac{1}{8R^2}U_a+\frac{\sin^2\alpha}{2r_a^2}T_a-\frac{1}{8r_a}T_a^2+\frac{1}{8R^2}U_b+\frac{\sin^2\beta}{2r_b^2}T_b-\frac{1}{8r_b}T_b^2\right)$$

$$F_{500}=y^5\left(\frac{\sin\alpha}{8R^2r_a}U_a+\frac{\sin^3\alpha}{2r_a^3}T_a-\frac{3\sin\alpha}{8r_a^2}T_a^2+\frac{\sin\beta}{8R^2r_b}U_b+\frac{\sin^3\beta}{2r_b^3}T_b-\frac{3\sin\beta}{8r_b^2}T_b^2\right)$$

$$F_{600}=y^6\left(\begin{array}{l}\frac{1}{16R^4}U_a+\frac{\sin^2\alpha}{8R^2r_a^2}U_a+\frac{\sin^4\alpha}{2r_a^4}T_a-\frac{1}{16R^2r_a}U_aT_a-\frac{3\sin^2\alpha}{4r_a^3}T_a^2+\frac{1}{16r_a^2}T_a^3\\+\frac{1}{16R^4}U_b+\frac{\sin^2\beta}{8R^2r_b^2}U_b+\frac{\sin^4\alpha}{2r_b^4}T_b-\frac{1}{16R^2r_b}U_bT_b-\frac{3\sin^2\beta}{4r_b^3}T_b^2+\frac{1}{16r_b^2}T_b^3\end{array}\right)$$

$$F_{020}=z^2\left(\frac{S_a}{2}+\frac{S_b}{2}\right)\text{; astigmatism}$$

$$F_{120}=yz^2\left(\frac{\sin\alpha}{2r_a}S_a+\frac{\sin\beta}{2r_b}S_b\right)\text{; astigmatic coma}$$

$$F_{220}=y^2z^2\left(\frac{1}{4R\rho}U_a+\frac{\sin^2\alpha}{2r_a^2}S_a-\frac{1}{4r_a}S_aT_a+\frac{1}{4R\rho}U_b+\frac{\sin^2\beta}{2r_b^2}S_b-\frac{1}{4r_b}S_bT_b\right)$$

$$F_{320}=y^3z^2\left(\frac{\sin\alpha}{4R\rho r_a}U_a+\frac{\sin^3\alpha}{2r_a^3}S_a-\frac{3\sin\alpha}{4r_a^2}S_aT_a+\frac{\sin\beta}{4R\rho r_b}U_b+\frac{\sin^3\beta}{2r_b^3}S_b-\frac{3\sin\beta}{4r_b^2}S_bT_b\right)$$

$$F_{420}=y^3z^2\left(\begin{array}{l}\frac{\sin^2\alpha}{4R\rho r_a^2}U_a+\frac{\sin^4\alpha}{2r_a^4}S_a-\frac{1}{8R\rho r_a^2}U_aT_a-\frac{1}{16R^2r_a}U_aS_a-\frac{3\sin^2\alpha}{2r_a^3}S_aT_a\\+\frac{3}{16r_a^2}S_aT_a^2+\frac{3}{16R^3\rho}U_a+\frac{\sin^2\beta}{4R\rho r_b^2}U_b+\frac{\sin^4\beta}{2r_b^4}S_b-\frac{1}{8R\rho r_b^2}U_bT_b\\-\frac{1}{16R^2r_b}U_bS_b-\frac{3\sin^2\beta}{2r_b^3}S_bT_b+\frac{3}{16r_b^2}S_bT_b^2+\frac{3}{16R^3\rho}U_b\end{array}\right)$$

$$F_{040}=z^4\left(\frac{1}{8\rho^2}S_a-\frac{1}{8r_a}S_a^2+\frac{1}{8\rho^2}S_b-\frac{1}{8r_b}S_b^2\right)$$

$$F_{140}=yz^4\left(\frac{\sin\alpha}{8\rho^2r_a}S_a-\frac{3\sin\alpha}{8r_a^2}S_a^2+\frac{\sin\beta}{8\rho^2r_b}S_b-\frac{3\sin\beta}{8r_b^2}S_b^2\right)$$

$$F_{240} = y^2 z^4 \begin{pmatrix} \frac{3}{16 r_a{}^2} S_a{}^2 T_a - \frac{1}{16\rho^2 r_a} S_a T_a + \frac{\sin^2\alpha}{8\rho^2 r_a{}^2} S_a - \frac{1}{8R\rho r_a} S_a U_a + \frac{1}{16R\rho^3} U_a \\ -\frac{3\sin^2\alpha}{4 r_a{}^3} S_a{}^2 + \frac{1}{8R^2\rho^2} U_a + \frac{3}{16 r_b{}^2} S_b{}^2 T_b - \frac{1}{16\rho^2 r_b} S_b T_b \\ + \frac{\sin^2\beta}{8\rho^2 r_b{}^2} S_b - \frac{1}{8R\rho r_b} S_b U_b + \frac{1}{16R\rho^3} U_b - \frac{3\sin^2\beta}{4 r_b{}^3} S_b{}^2 + \frac{1}{8R^2\rho^2} U_b \end{pmatrix}$$

$$F_{011} = zz_a\left(-\frac{1}{r_a}\right) + zz_b\left(-\frac{1}{r_b}\right)$$

$$F_{111} = yzz_a\left(-\frac{\sin\alpha}{r_a{}^2}\right) + yzz_b\left(-\frac{\sin\beta}{r_b{}^2}\right)$$

$$F_{211} = y^2 zz_a\left(\frac{1}{2 r_a{}^2} T_a - \frac{\sin^2\alpha}{r_a{}^3}\right) + y^2 zz_b\left(\frac{1}{2 r_b{}^2} T_b - \frac{\sin^2\beta}{r_b{}^3}\right)$$

$$F_{311} = y^3 zz_a\left(\frac{3\sin\alpha}{2 r_a{}^3} T_a - \frac{\sin^3\alpha}{r_a{}^4}\right) + y^3 zz_b\left(\frac{3\sin\beta}{2 r_b{}^3} T_a - \frac{\sin^3\beta}{r_b{}^4}\right)$$

$$F_{411} = y^4 zz_a\left(\frac{1}{8R^2 r_a{}^2} U_a - \frac{\sin^4\alpha}{r_a{}^5} + \frac{3\sin^2\alpha}{r_a{}^4} T_a - \frac{3}{8 r_a{}^3} T_a{}^2\right)$$
$$+ y^4 zz_b\left(\frac{1}{8R^2 r_b{}^2} U_b - \frac{\sin^4\beta}{r_b{}^5} + \frac{3\sin^2\beta}{r_b{}^4} T_b - \frac{3}{8 r_b{}^3} T_b{}^2\right)$$

$$F_{002} = z_a{}^2\left(\frac{1}{2 r_a}\right) + z_b{}^2\left(\frac{1}{2 r_b}\right)$$

$$F_{102} = yz_a{}^2\left(\frac{\sin\alpha}{2 r_a{}^2} + \frac{\sin\beta}{2 r_b{}^2}\right) + yz_b{}^2\left(\frac{\sin\beta}{2 r_b{}^2}\right)$$

$$F_{202} = y^2 z_a{}^2\left(\frac{\sin^2\alpha}{2 r_a{}^3} - \frac{1}{4 r_a{}^2} T_a\right) + y^2 z_b{}^2\left(\frac{\sin^2\beta}{2 r_b{}^3} - \frac{1}{4 r_b{}^2} T_b\right)$$

$$F_{302} = y^3 z_a{}^2\left(\frac{\sin^3\alpha}{2 r_a{}^4} - \frac{3\sin\alpha}{4 r_a{}^3} T_a\right) + y^3 z_b{}^2\left(\frac{\sin^3\beta}{2 r_b{}^4} - \frac{3\sin\beta}{4 r_b{}^3} T_b\right)$$

$$F_{402} = y^4 z_a^{\ 2}\left(\frac{\sin^4\alpha}{2r_a^{\ 5}} - \frac{1}{16R^2 r_a^{\ 2}}U_a - \frac{3\sin^2\alpha}{2r_a^{\ 4}}T_a - \frac{3}{16r_a^{\ 3}}T_a^{\ 2}\right)$$
$$+y^4 z_b^{\ 2}\left(\frac{\sin^4\beta}{2r_b^{\ 5}} - \frac{1}{16R^2 r_b^{\ 2}}U_b - \frac{3\sin^2\beta}{2r_b^{\ 4}}T_b - \frac{3}{16r_b^{\ 3}}T_b^{\ 2}\right)$$

$$F_{031} = z^3 z_a\left(\frac{1}{2r_a^{\ 2}}S_a\right) + z^3 z_b\left(\frac{1}{2r_b^{\ 2}}S_b\right)$$

$$F_{131} = yz^3 z_a\left(\frac{3\sin\alpha}{2r_a^{\ 3}}S_a\right) + yz^3 z_b\left(\frac{3\sin\beta}{2r_b^{\ 3}}S_b\right)$$

$$F_{231} = y^2 z^3 z_a\left(\frac{1}{4R\rho r_a^{\ 2}}U_a + \frac{3\sin^2\alpha}{r_a^{\ 4}}S_a - \frac{3}{4r_a^{\ 3}}S_a T_a\right) + y^2 z^3 z_b\left(\frac{1}{4R\rho r_b^{\ 2}}U_b + \frac{3\sin^2\beta}{r_b^{\ 4}}S_b - \frac{3}{4r_b^{\ 3}}S_b T_b\right)$$

$$F_{042} = z^4 z_a^{\ 2}\left(\frac{3}{4r_a^{\ 4}}S_a - \frac{1}{16r^2 r_a^{\ 2}}S_a + \frac{3}{16r_a^{\ 3}}S_a^{\ 2}\right) + z^4 z_b^{\ 2}\left(\frac{3}{4r_b^{\ 4}}S_b - \frac{1}{16r^2 r_b^{\ 2}}S_b + \frac{3}{16r_b^{\ 3}}S_b^{\ 2}\right)$$

$$F_{013} = zz_a^{\ 3}\left(\frac{1}{2r_a^{\ 3}}\right) + zz_b^{\ 3}\left(\frac{1}{2r_b^{\ 3}}\right)$$

$$F_{022} = z^2 z_a^{\ 2}\left(-\frac{1}{2r_a^{\ 3}} - \frac{1}{4r_a^{\ 2}}S_a\right) + z^2 z_b^{\ 2}\left(-\frac{1}{2r_b^{\ 3}} - \frac{1}{4r_b^{\ 2}}S_b\right)$$

$$F_{122} = yz^2 z_a^{\ 2}\left(-\frac{3\sin\alpha}{2r_a^{\ 4}} - \frac{3\sin\alpha}{4r_a^{\ 3}}S_a\right) + yz^2 z_b^{\ 2}\left(-\frac{3\sin\beta}{2r_b^{\ 4}} - \frac{3\sin\beta}{4r_b^{\ 3}}S_b\right)$$

$$F_{222} = y^2 z^2 z_a^{\ 2}\left(\frac{3}{4r_a}T_a + \frac{3}{8r_a^{\ 3}}S_a T_a - \frac{1}{8Rrr_a^{\ 2}}U_a - \frac{3\sin^2\alpha}{2r_a^{\ 4}}S_a - \frac{3\sin^2\alpha}{r_a^{\ 5}}\right)$$
$$+y^2 z^2 z_b^{\ 2}\left(\frac{3}{4r_b}T_b + \frac{3}{8r_b^{\ 3}}S_b T_b - \frac{1}{8Rrr_b^{\ 2}}U_b - \frac{3\sin^2\beta}{2r_b^{\ 4}}S_b - \frac{3\sin^2\beta}{r_b^{\ 5}}\right)$$

Holographic Gratings

Holographic gratings are generated by creating a mask using the diffraction pattern of two interfering laser beams from points C and D at distances of r_c and r_d, and angles of γ and δ. If the recording wavelength of the laser is λ_0 then there will be n fringes between O and P and the path length for n fringes at λ_0 is

$$n\lambda_0 = \left(\langle CP\rangle + \langle PD\rangle\right) - \left(\langle CO\rangle + \langle OD\rangle\right)$$

with, if $\gamma = \delta$, a d spacing of

$$d = \frac{\lambda_0}{2\sin\delta}.$$

Ignoring the second term which is a constant and plugging this in to our original path length function we get

$$F = \langle AP\rangle + \langle PB\rangle + m\lambda n = \langle AP\rangle + \langle PB\rangle + \frac{m\lambda}{\lambda_0}\left(\langle CP\rangle + \langle PD\rangle\right)$$

which on expansion yields addition terms to our F_{ijk}. F_{100} would become for example

$$F_{100} = y\left(-\sin\alpha - \sin\beta + \frac{m\lambda}{\lambda_0}(-\sin\gamma - \sin\delta)\right)$$

Which if our angles are equal reduces to the grating equation.

Appendix 2 Exit Slit Position

Appendix 3 Mono.prg

```
#-----------------------------------------------------------------------#
# MONO.PRG                                                              #
# Monochromator control script for BL 8-1                               #
# 3/10/1999 - 3/22/2000                                                 #
#-----------------------------------------------------------------------#
DEVICE MONO,GRATING,XSLIT
DEVICE_A XSLIT_A,GRATING_A,MONO_A
DEVICE_R XSLIT_R,GRATING_R,MONO_R
DEVICE_L XSLIT_L,GRATING_L
DEVICE_DP1 MONO_DP1,GRATING_DP1,XSLIT_DP1       #lines per mm
DEVICE_DP2 MONO_DP2,GRATING_DP2,XSLIT_DP2       #zero order position
DEVICE_DP3 MONO_DP3,GRATING_DP3,XSLIT_DP3       #sinbar length
DEVICE_DP4 MONO_DP4,GRATING_DP4,XSLIT_DP4       #opening angle phi
DEVICE_DP5 MONO_DP5,GRATING_DP5,XSLIT_DP5       #order
DEVICE_DP6 MONO_DP6,GRATING_DP6,XSLIT_DP6       #expected grating position
DEVICE_DP7 MONO_DP7,GRATING_DP7,XSLIT_DP7       #expected xslit position
DEVICE_DP8 MONO_DP8,GRATING_DP8,XSLIT_DP8
DEVICE_DP9 MONO_DP9
DEVICE_DP10 MONO_DP10
DEVICE_DP11 MONO_DP11

DOUBLE a1,a2,al,bt,c0,c1,c2,ca,CALB,cb,CAMP,cx,cy,cz,d2,db,e,gg,gp,lp
DOUBLE od,ph2,ph,r,rc0,rc1,rc2,TEST,x1,x2,y,zp
DOUBLE a00,a01,a02,a10,a11,a12,a20,a21,a22,b0,b1,b2,dbn1,dbn2,dbn3
DOUBLE dbo1,dbo2,det0,det1,det2,detc,en1,en2,eo1,eo2,gpo1,gpo2,gpo3
DOUBLE sb,lm,ga,gr,x,qc0,qc1,qc2
DOUBLE z,a,b,b1,c,d1,d3,r1

BEGIN main
 CALL assign_constants                  # fill up constants
 ASSIGN e MONO_A                        #
 CALL calc_xslit                        # calculate pos. of xslit to x
 ASSIGN x1 x                            # save xslit position to x1
 ASSIGN e MONO_R                        # copy requested energy to e
 CALL calc_grating                      # calculate the position of grating
 .GT. y CALB 0
 IF y
   CALL calc_coeff
 END_IF
 .GT. y CAMP 0
 IF y
   CALL calc_compgrat
 END_IF
 ASSIGN GRATING_R gp                    # copy to requested pos. for grating
 ASSIGN gr GRATING_R                    # copy grating req. pos to gr
 CALL calc_xslit                        # calculate new position of xslit
 SUB x2 x x1                            # find the diff. in xslit positions
 move_abs_a { GRATING, GRATING_R }      # move crystal, absolute async.
 IF (TEST.GT.0)
  move_rel_a { XSLIT, x2 }              # move table relative, async.
 END_IF

 device_wait { MONO }                   # wait for them both to complete

 CALL calc_cm                           # calculate the new energy
END
```

```
SUBROUTINE calc_cm
# calc_cm calculate position of combination motor from critical motor
# MONO_A = 12398.4244 /(2e7*cos(phi/2)sin(alpha +phi/2)/(lines*order))
# where alpha = -phi/2 + arctan((zop - M)/l)
# if not using the geometrical transfer function call calc_compenergy
 CALL assign_constants
 ASSIGN gp GRATING_A
 SUB al zp gp
 DIV al al sb
 ATAN al al
 SIN al al
 MUL al al 20000000
 DIV al al lp
 DIV al al od
 COS b a
 MUL al al b
 DIV e 12398.4244 al

 .GT. y CAMP 0
 IF y
   CALL calc_compenergy
 END_IF

 ASSIGN MONO_A e
RETURN

SUBROUTINE calc_mm
# calc_mm calculate position of critical motor from combination motor
# if not using the geometrical transfer functions RETURN
# calculates the new zero order position for a change in energy
# zopnew = zopold +gpold -gpnew
 CALL assign_constants

 .GT. y CAMP 0
 IF y
   RETURN
 END_IF

 ASSIGN e MONO_A
 CALL calc_grating
 SUB gg GRATING_A gp
 ADD zp zp gg
 ASSIGN GRATING_DP2 zp
RETURN

SUBROUTINE calc_ac
# calc_ac calculate position of other motors from critical motor
 CALL assign_constants
 ASSIGN gp GRATING_L
 CALL calc_xslit
 ASSIGN x1 x
 ASSIGN gp GRATING_A
 CALL calc_xslit
 SUB x1 x x1

 ADD x XSLIT_L x1
 SUB gr x XSLIT_A
 move_rel XSLIT gr
RETURN

SUBROUTINE calc_compgrat
# Calculates the grating position from the second order polynomial
# where gp = c0 + (psi*(c1 + psi*c2))
# and psi = alpha + ph/2
  CALL assign_constants
  ASSIGN cx c0
```

```
  ASSIGN cy c1
  ASSIGN cz c2

  .EQ. a1 lp 822
  IF a1
    ASSIGN cx rc0
    ASSIGN cy rc1
    ASSIGN cz rc2
  END_IF

  .EQ. a1 lp 2400
  IF a1
    ASSIGN cx qc0
    ASSIGN cy qc1
    ASSIGN cz qc2
  END_IF

  CALL calc_alpha
  ADD db al ph2
  MUL gp db cz
  ADD gp gp cy
  MUL gp gp db
  ADD gp gp cx
RETURN



SUBROUTINE calc_coeff
# calculates the coefficients for moving the monochromator from
# user supplied data, then resets the switch to zero
# the coefficients are calculated by solving three simultaneous
# equations using Cramers rule
  CALL assign_constants
  ASSIGN e eo1
  CALL calc_alpha
  ADD dbo1 al ph2
  ASSIGN e eo2
  CALL calc_alpha
  ADD dbo2 al ph2
  ASSIGN e en1
  CALL calc_alpha
  ADD dbn1 al ph2
  ASSIGN e en2
  CALL calc_alpha
  ADD dbn2 al ph2

  .EQ. y c0 0
  .EQ. a1 lp 288
  .AND. a1 y a1
  IF a1
    CALL assign_288
  END_IF

  .EQ. y rc0 0
  .EQ. a1 lp 822
  .AND. a1 y a1
  IF a1
    CALL assign_822
  END_IF

  .EQ. y qc0 0
  .EQ. a1 lp 2400
  .AND. a1 y a1
  IF a1
    CALL assign_2400
  END_IF
```

```
  ASSIGN cx c0
  ASSIGN cy c1
  ASSIGN cz c2

  .EQ. a1 lp 822
  IF a1
    ASSIGN cx rc0
    ASSIGN cy rc1
    ASSIGN cz rc2
  END_IF

  .EQ. a1 lp 2400
  IF a1
    ASSIGN cx qc0
    ASSIGN cy qc1
    ASSIGN cz qc2
  END_IF

  ASSIGN dbn3 0
  ASSIGN gpo3 zp
  MUL gpo1 dbo1 cz
  ADD gpo1 gpo1 cy
  MUL gpo1 gpo1 dbo1
  ADD gpo1 gpo1 cx
  MUL gpo2 dbo2 cz
  ADD gpo2 gpo2 cy
  MUL gpo2 gpo2 dbo2
  ADD gpo2 gpo2 cx
# Fill matrices
  ASSIGN a01 dbn1
  ASSIGN a11 dbn2
  ASSIGN a21 dbn3
  ASSIGN b0 gpo1
  ASSIGN b1 gpo2
  ASSIGN b2 gpo3
  ASSIGN a00 1
  ASSIGN a10 1
  ASSIGN a20 1
  MUL a02 a01 a01
  MUL a12 a11 a11
  MUL a22 a21 a21
# calculate determinant C
  MUL a1 a11 a22       #a1=a11*a22
  MUL a2 a21 a12       #a2=a21*a12
  SUB detc a1 a2       #detc=a11*a22-a21*a12
  MUL detc detc a00    #detc=a00(a11a22-a21a12)
  MUL a1 a10 a22       #a1=a10*a22
  MUL a2 a20 a12       #a2=a20*a12
  SUB a1 a1 a2         #a1=a10*a22-a20*a12
  MUL a1 a1 a01                #a1=a01(a10a22-a20a12)
  SUB detc detc a1     #detc=a00(a11a22-a21a12)-a01(a10a22-a20a12)
  MUL a1 a10 a21       #a1=a10*a21
  MUL a2 a20 a11       #a2=a20*a11
  SUB a1 a1 a2         #a1=a10a21-a20a11
  MUL a1 a1 a02                #a1=a02(a10a21-a20a11)
  ADD detc detc a1     #detc=.....
# Reassign elements
  ASSIGN b0 a00
  ASSIGN b1 a10
  ASSIGN b2 a20
  ASSIGN a00 gpo1
  ASSIGN a10 gpo2
  ASSIGN a20 gpo3
# calculate determinant 0
  MUL a1 a11 a22        #a1=a11*a22
```

```
  MUL a2 a21 a12        #a2=a21*a12
  SUB det0 a1 a2        #det0=a11*a22-a21*a12
  MUL det0 det0 a00     #det0=a00(a11a22-a21a12)
  MUL a1 a10 a22        #a1=a10*a22
  MUL a2 a20 a12        #a2=a20*a12
  SUB a1 a1 a2          #a1=a10*a22-a20*a12
  MUL a1 a1 a01         #a1=a01(a10a22-a20a12)
  SUB det0 det0 a1      #det0=a00(a11a22-a21a12)-a01(a10a22-a20a12)
  MUL a1 a10 a21        #a1=a10*a21
  MUL a2 a20 a11        #a2=a20*a11
  SUB a1 a1 a2          #a1=a10a21-a20a11
  MUL a1 a1 a02         #a1=a02(a10a21-a20a11)
  ADD det0 det0 a1      #det0=.....
# Reassign elements
  ASSIGN a00 b0
  ASSIGN a10 b1
  ASSIGN a20 b2
  ASSIGN b0 a01
  ASSIGN b1 a11
  ASSIGN b2 a21
  ASSIGN a01 gpo1
  ASSIGN a11 gpo2
  ASSIGN a21 gpo3
# calculate determinant 1
  MUL a1 a11 a22        #a1=a11*a22
  MUL a2 a21 a12        #a2=a21*a12
  SUB det1 a1 a2        #det1=a11*a22-a21*a12
  MUL det1 det1 a00     #det1=a00(a11a22-a21a12)
  MUL a1 a10 a22        #a1=a10*a22
  MUL a2 a20 a12        #a2=a20*a12
  SUB a1 a1 a2          #a1=a10*a22-a20*a12
  MUL a1 a1 a01         #a1=a01(a10a22-a20a12)
  SUB det1 det1 a1      #det1=a00(a11a22-a21a12)-a01(a10a22-a20a12)
  MUL a1 a10 a21        #a1=a10*a21
  MUL a2 a20 a11        #a2=a20*a11
  SUB a1 a1 a2          #a1=a10a21-a20a11
  MUL a1 a1 a02         #a1=a02(a10a21-a20a11)
  ADD det1 det1 a1      #det1=.....
# Reassign elements
  ASSIGN a01 b0
  ASSIGN a11 b1
  ASSIGN a21 b2
  ASSIGN a02 gpo1
  ASSIGN a12 gpo2
  ASSIGN a22 gpo3
# calculate determinant 2
  MUL a1 a11 a22        #a1=a11*a22
  MUL a2 a21 a12        #a2=a21*a12
  SUB det2 a1 a2        #det2=a11*a22-a21*a12
  MUL det2 det2 a00     #det2=a00(a11a22-a21a12)
  MUL a1 a10 a22        #a1=a10*a22
  MUL a2 a20 a12        #a2=a20*a12
  SUB a1 a1 a2          #a1=a10*a22-a20*a12
  MUL a1 a1 a01         #a1=a01(a10a22-a20a12)
  SUB det2 det2 a1      #det2=a00(a11a22-a21a12)-a01(a10a22-a20a12)
  MUL a1 a10 a21        #a1=a10*a21
  MUL a2 a20 a11        #a2=a20*a11
  SUB a1 a1 a2          #a1=a10a21-a20a11
  MUL a1 a1 a02         #a1=a02(a10a21-a20a11)
  ADD det2 det2 a1      #det2=.....
# solve for coefficients
  .EQ. a1 lp 288
  IF a1
    DIV c0 det0 detc     #c0=det0/detc
    DIV c1 det1 detc     #c1=det1/detc
    DIV c2 det2 detc     #c2=det2/detc
```

```
    ASSIGN MONO_DP1 c0
    ASSIGN MONO_DP2 c1
    ASSIGN MONO_DP3 c2
    ASSIGN MONO_DP11 0
  END_IF
  .EQ. a1 lp 822
  IF a1
    DIV rc0 det0 detc
    DIV rc1 det1 detc
    DIV rc2 det2 detc
    ASSIGN MONO_DP4 rc0
    ASSIGN MONO_DP5 rc1
    ASSIGN MONO_DP6 rc2
    ASSIGN MONO_DP11 0
  END_IF
  .EQ. a1 lp 2400
  IF a1
    DIV qc0 det0 detc
    DIV qc1 det1 detc
    DIV qc2 det2 detc
    ASSIGN MONO_DP7 qc0
    ASSIGN MONO_DP8 qc1
    ASSIGN MONO_DP9 qc2
    ASSIGN MONO_DP11 0
  END_IF
RETURN

SUBROUTINE assign_288
  ASSIGN c0 1825
  ASSIGN c1 -6639.393096
  ASSIGN c2 -6.979122474
RETURN

SUBROUTINE assign_822
  ASSIGN rc0 1700
  ASSIGN rc1 -6554.382577
  ASSIGN rc2 -15.2919105
RETURN

SUBROUTINE assign_2400
  ASSIGN qc0 1769
  ASSIGN qc1 -6601.198611
  ASSIGN qc2 -10.71624832
RETURN


SUBROUTINE calc_alpha
#calculates alpha and beta
  CALL assign_constants
  MUL bt lp od          #bt=lines*order
  MUL bt bt .001239854  #bt=lines*order*.00123984244
  DIV bt bt 2           #bt=lp*n*.00123984244/2
  DIV bt bt e           #bt=lp*n*c/(2*energy)
  COS a1 ph2            #a1=cos(phi/2)
  DIV bt bt a1          #bt=lp*n*c/(2*e*cos(phi/2)
  ASIN bt bt            #beta=asin(lp*n*c/(2*e*cos(phi/2)))
  SUB al bt ph2         #alpha=beta-phi/2
  ADD bt bt ph2
RETURN

SUBROUTINE calc_compenergy
#calculates the Back transfer function for the second order
#polynomial using the quadratic equation
  CALL assign_constants
  ASSIGN cx c0
  ASSIGN cy c1
```

```
  ASSIGN cz c2

  .EQ. a1 lp 822
  IF a1
    ASSIGN cx rc0
    ASSIGN cy rc1
    ASSIGN cz rc2
  END_IF

  .EQ. a1 lp 2400
  IF a1
    ASSIGN cx qc0
    ASSIGN cy qc1
    ASSIGN cz qc2
  END_IF

  SUB a1 cx gp
  MUL a1 a1 cz
  MUL a1 a1 4
  MUL a2 cy cy
  SUB a1 a2 a1
  SQRT a1 a1
  SUB a1 0 a1
  SUB a1 a1 cy
  DIV a1 a1 2
  DIV a1 a1 cz
  SIN a1 a1             #a1=sin(al)
  COS a2 ph2            #a2=cos(phi/2)
  DIV d2 20000000 lp    #d2=20,000,000/lines(in Angstroms)
  MUL e od 12398.4244   #e=n*12398.4244
  DIV e e d2            #e=n*12398.4244/2d
  DIV e e a1            #e=n*12398.4244/(2d*sin(al+phi/2))
  DIV e e a2            #e=n*12398.4244/(2d*sin(al+phi/2)*cos(phi/2))
RETURN


SUBROUTINE calc_xslit
#this calculates the position of the exit slit for any standard TGM os SGM
#beam line (not 8-1)
 MUL c lp .00123984244
 DIV c c 2
 DIV c c e
 DIV a ph 2
 COS b a
 DIV c c b
 ASIN c c
 ADD a1 c a
 SUB b1 c a
 MUL d1 r1 r
 COS cb b1
 COS ca a1
 MUL d1 d1 cb
 MUL d1 d1 cb
 ADD d2 ca cb
 MUL d2 d2 r1
 MUL d3 ca ca
 MUL d3 d3 r
 SUB d3 0 d3
 ADD d2 d2 d3
 DIV x d1 d2
RETURN

SUBROUTINE calc_grating
#calculates the geometrical forward transfer function
 DIV lm 12398.4244 e
```

```
 MUL al lm od
 MUL al al lp
 DIV al al 20000000.0
 DIV a  ph 2
 COS b  a
 DIV al al b
 ASIN al al
 TAN gp al
 MUL gp gp sb
 SUB gp zp gp
RETURN

SUBROUTINE assign_constants
 ASSIGN lp GRATING_DP1          #lines per millimeter
 ASSIGN zp GRATING_DP2          #zero order position
 ASSIGN sb 381000               #sin-bar length
 ASSIGN ph GRATING_DP3          #opening angle phi
 DIV ph2 ph 2                   #phi/2
 ASSIGN od GRATING_DP4          #order
 ASSIGN eo1 GRATING_DP5         #first energy under old calibration
 ASSIGN en1 GRATING_DP6         #first energy under new calibration
 ASSIGN eo2 GRATING_DP7         #second energy under old calibration
 ASSIGN en2 GRATING_DP8         #second energy under new calibration
 ASSIGN r  XSLIT_DP1
 ASSIGN r1 XSLIT_DP2
 ASSIGN c0 MONO_DP1
 ASSIGN c1 MONO_DP2
 ASSIGN c2 MONO_DP3
 ASSIGN rc0 MONO_DP4
 ASSIGN rc1 MONO_DP5
 ASSIGN rc2 MONO_DP6
 ASSIGN qc0 MONO_DP7
 ASSIGN qc1 MONO_DP8
 ASSIGN qc2 MONO_DP9
 ASSIGN CAMP MONO_DP10          #use calibration to move mono
 ASSIGN CALB MONO_DP11          #calibrate mono using new coeff
RETURN
```