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Theory of a Modified Wadsworth Monochromator Matched to a Low Energy Storage Ring Source*

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ABSTRACT

The concave diffraction grating in the Wadsworth mounting has been popular with synchrotron radiation spectroscopists because of its use of parallel light. This is well matched to experimental stations which are a great distance away of the source as would be the case in using a high energy synchrotron. For low energy storage rings the working distance is quite small and in this case it is appropriate to use a collimating mirror. Large collection angles are possible with this arrangement and reasonable resolution can be obtained using spherical surfaces. Astigmatism is much lower than for Rowland circle mountings. These questions are analyzed using an optical path function development and calculations are presented which include the aberrations both in the two optics and those caused by the large extension of the source in the direction of the radiation emission.

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1. Introduction

It seems to be generally agreed that for low energy synchrotron radiation studies it is preferable to use a storage ring of low energy. Among the advantages of this approach are the much reduced radiation shielding requirements and the corresponding shorter working distances. The resulting collection angles can be quite large and it becomes necessary to address the question of how to design optics which can exploit the rather special geometry which arises.

Large angle optics will naturally tend to be normal incidence optics and we may have to accommodate a source geometry comprising a small source size with an angular spread of about 5-10mr in the vertical and perhaps 50-100mr in the horizontal. For high resolution work one would use an instrument with an entrance slit but for moderate resolution with a small source there are many advantages in using the source itself as entrance slit. Usually the source is narrower in the vertical direction so that we naturally choose a vertical plane of dispersion. The largest angular spread is therefore perpendicular to the plane of the instrument.

We will try to write a general discussion of this class of instrument but we will also keep in mind a concrete example: that of a beamline presently under construction at the NSLS VUV storage ring at Brookhaven. For this case the total angular acceptance is 8mr(V)x55mr(H). The electron beam size is 0.2mm(V)x1.0mm(H) and the first mirror of the beamline is 2861mm from the source.

2. Design Layout

Some types of constant deviation monochromator which could be considered are the following:

1. McPherson 225 (3m say).(1,2)
2. Pouey unsymmetrical VUV device.(3)
3. Monk-Gillieson.(4,5,6)
4. Wadsworth.(7,8)

In all cases it is necessary to make some arrangement to ensure that the light emerging from the monochromator is travelling away from the storage ring. In cases 1 and 2 it is necessary to provide a plane mirror whose only purpose is to fold the 'vee' shape of the configuration into a zig-zag shape (Fig. 1). For case 3 this happens naturally and for case 4 it is necessary to provide a collimator so that, again, the folding occurs naturally.

The choice between these alternatives depends to some extent on the application. However, without too much loss of generality we can assume that a small focal spot is desirable and also that we wish to remain within conventional grating technology. We, thus, forswear the use of aspheric or holographically corrected gratings.

The small focal spot (low astigmatism) argument favors alternatives 3 and 4. The Wadsworth has the further advantage that since the light between the mirror and the grating is parallel the mirror/grating distance can be anything and the two arm lengths can be chosen independently. The Monk-Gillieson scheme is also quite flexible and is said (6) to have astigmatism equivalent to a Seya-Namioka monochromator with an elliptical grating. However, when configured for best aberration cancelling (6) it has the

disadvantage of crossover geometry. There are possibilities for designing around this but the whole system is more in the nature of a development project than the other schemes. An instrument of this kind is under construction for use at the BESSY storage ring. However, the geometry there is somewhat different than at Brookhaven. The working distance is about twice as large and this gives rise to correspondingly larger optics. The use of a plane grating is thus much more compelling.

These general arguments, at least for the case of Brookhaven, lead us to choose the Wadsworth design and we now proceed to develop the theory of this. Our intention is to show that one can have a design which has good astigmatism properties and has source limited resolution over the whole spectral range. We shall see that for the Brookhaven source geometry we can, indeed, have system aberrations which are small compared to the effect of the source size.

3. Preliminary Theory

Before we develop the theory of the mirror/grating combination we need to recall the simple theory of the Wadsworth mounting. It is well known that the focussing term C_{20} of the optical path function expansion of the concave grating of radius R is given by

$$C_{20} = \frac{1}{2} \left[\left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \right] \quad (1)$$

Where α and β are the angles of incidence and diffraction and r and r' are the object and image distances. The grating is in focus for the wavelength corresponding to α and β if $C_{20}=0$. This is the case if either the Rowland Circle condition is satisfied or

$$r = \infty, \quad r' = \frac{R \cos^2 \beta}{\cos \alpha + \cos \beta}. \quad (2)$$

(2) defines the Wadsworth mounting. Since we are interested in a constant deviation monochromator we will rotate the grating keeping the inward and outward directions fixed. In other words we impose the condition

$$\alpha - \beta = 2\theta \quad (3)$$

Where 2θ is the angle between the inward and outward direction and we are using the usual sign convention.⁽⁹⁾ The wavelength λ_w for which $\rho = 0$ (hence $\alpha = 2\theta$) is known as the Wadsworth wavelength. We shall see later that the grating is perfectly stigmatic at λ_w . The value of r' needed to be in focus at λ_w is given by (2) as

$$r'_w = \frac{R}{1 + \cos 2\theta} \quad (4)$$

The usefulness of the Wadsworth mounting lies in the fact that the main aberrations, especially coma and astigmatism, vary slowly with wavelength and are zero at λ_w and small over a range of wavelengths close to λ_w . We thus want λ_w near the center of our working range. Now the grating equation tells us

$$m\lambda = d(\sin\alpha + \sin\beta) \quad (5)$$

where m is the order and d the groove spacing. So for $m = 1$

$$\lambda_w = d \sin 2\theta \quad (6)$$

For the Brookhaven design $1/d = 2400$ gr/mm and $\theta = 6^\circ$ giving $\lambda_w = 866\text{\AA}$.

We can now plot out the r' values needed for focus. This is shown for the Brookhaven case in Fig. 2. Assuming that the only realistic mechanical system we can design will give a linear correction to the focal distance we get the fit shown in Fig. 2. From this we can compute the length of a pivot arm. Once this is done we know the proper position for the slit and the actual position of the grating for any wavelength. It turns out for the Brookhaven parameters that with the correction the defocus error is always less than the source size limit.

4. Theory

We now consider the configuration illustrated in Fig. 3. For the time being we assume a point source illuminating a spherical mirror which is set to work as a collimator. Nominally parallel light from the mirror illuminates the spherical grating and is then focussed in the neighborhood of the slit. We adopt an optical path function development and simply write the optical path function of the two optics as the sum of the separate optical path functions. This procedure is valid provided the aperture co-ordinates for the second optic can be derived with sufficient accuracy from those of the first optic by means of the paraxial (' $\sin \theta \approx \theta$ ') approximation. Since the distance between the optics is small compared to the object and image distances in the present case we expect that imperfections in collimation by the mirror (aberrations) will not significantly affect the computed positions of ray intersections with the grating aperture. The summing of the optical paths is therefore valid. Our use of a point source eliminates from the power series all terms that contain the field co-ordinate z and we truncate the series after the third order terms in w and l . This is equivalent to neglecting spherical aberration compared to coma and defocus which would not normally be appropriate. However, we justify it in this case because $k_{\max} \sim 7w_{\max}$ and the rulings are parallel to the long direction of the grating blank.

From Fig. 3 one can see the co-ordinate system. It is identical as far as possible to that of Namioka.⁽¹⁰⁾ We now write down the overall optical path function W in a fairly general form

$$\begin{aligned}
W = & r_1 + r'_1 + \frac{1}{2} (T_1 + T'_1) w_1^2 + \frac{1}{2} (S_1 + S'_1) k_1^2 \\
& + \frac{1}{2} \left[\frac{\sin \theta}{r_1} S_1 + \frac{\sin(-\theta)}{r'_1} S'_1 \right] w_1 k_1^2 + \frac{1}{2} \left[\frac{\sin \theta}{r_1} T_1 + \frac{\sin(-\theta)}{r'_1} T'_1 \right] w_1^3 \\
& + r_2 + r'_2 + (\sin \alpha + \sin \beta - \frac{m\lambda}{d}) w_2 \\
& + \frac{1}{2} (T_2 + T'_2) w_2^2 + \frac{1}{2} (S_2 + S'_2) k_2^2 \\
& + \frac{1}{2} \left[\frac{\sin \alpha_2}{r_2} S_2 + \frac{\sin \beta_2}{r'_2} S'_2 \right] w_2 k_2^2 + \frac{1}{2} \left[\frac{\sin \alpha_2}{r_2} T_2 + \frac{\sin \beta_2}{r'_2} T'_2 \right] w_2^3 \\
& + \text{HOT}
\end{aligned} \tag{6}$$

$$\text{where } T(\alpha, r) = \frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \quad \text{and } S(\alpha, r) = \frac{1}{r} - \frac{\cos \alpha}{R}$$

Subscript 1 refers to the mirror and subscript 2 to the grating. Unprimed variables refer to ingoing rays and primed variables to outgoing ones. We have specialized the grating terms to the mirror case by putting $\alpha = \theta$, $\beta = -\theta$. The various terms can be associated with particular aberrations as follows:

- $C_{00} k^0 w^0$ - principle ray (constant) term
- $C_{10} w$ - grating equation term
- $C_{20} w^2$ - focus
- $C_{02} k^2$ - astigmatism (focus perpendicular to symmetry plane)
- $C_{30} w^3$ - tangential coma.
- $C_{12} w k^2$ - sagittal coma

Note that because of the symmetry plane there are no terms in odd powers of k . We can now feed in the specifics of the present configuration and achieve some simplification of (6). Since the mirror is set as a collimator r'_1 and r_2

are both very large so terms in $\frac{1}{r_1'}$ and $\frac{1}{r_2'}$ drop out. Furthermore, the mirror is properly focussed in the tangential plane so $T_1 + T_1' = 0$ i.e. $r_1 = \frac{1}{2} R_1 \cos \theta$. Since light from the mirror is parallel we have from Fig. 3 that $w_1 = w_2 = w$ (say) and similarly $\ell_1 = -\ell_2 = \ell$. We are considering the wavelength λ which satisfies the grating equation so that term drops out. We are also interested mainly in the difference between W for a ray and W for the principle ray so we may speak of this as the aberrant optical path ΔW and drop the constant terms.

$$\begin{aligned} \Delta W = & \frac{\tan \theta \sin \theta}{R_1} \ell^2 + \frac{\sin \theta}{2r_1} (S_1 \ell^2 + T_1 w^2) w \\ & + \frac{1}{2} (T_2 + T_2') w + \frac{1}{2} (S_2 + S_2') \ell^2 - \frac{\sin 2\theta}{2r_2'} (S_2' \ell + T_2' w) w + \text{HOT} \end{aligned} \quad (7)$$

The usefulness of this expansion lies in the fact that one can use it to calculate ray aberrations that is the displacement from the paraxial focus, of a ray arriving at the image plane. The calculation shows clearly how each aberration contributes to the aberration blurr. The ray displacements Δy and Δx (parallel and perpendicular to the plane of Fig. 3 respectively) are given by (11)

$$\Delta y = \frac{r_2'}{\cos \theta} \frac{\partial(\Delta W)}{\partial w} \quad (8)$$

$$\Delta x = r_2' \frac{\partial(\Delta W)}{\partial \ell} \quad (9)$$

5. Interpretation

We can see qualitatively how the system will work from (7). The mirror contributes a fixed amount of astigmatism and coma which we can picture best by looking at the ray trace. This is shown in Fig. 4 for the Brookhaven

mirror for a point source at the tangential focus. (To visualize this we have reversed the mirror and traced incoming parallel rays back to an aberrated image at the tangential focus). We see astigmatism (the point is imaged as a line) and coma (the line is curved). The length of the line and the sag of the curve can be calculated using (8) and (9) and the appropriate terms of (7). eg.

$$\text{full line length} = \sin^2 \theta \cdot 2d_{\max} \quad (10)$$

(Here we have also assumed that $r_1 = \frac{1}{2} R_1 \cos \theta$)

$$\text{Sag} = \frac{1}{2} \tan^2 \theta s_1 \kappa_{\max}^2 \quad (11)$$

These give the right answer in the present case because the astigmatism is small. A more general form of (11) which includes the case of large astigmatism for a toroidal mirror of minor radius ρ is often useful: (12)

$$\text{Sag} = \frac{r_1' \kappa_{\max}^2 \sin \theta}{2\rho} \left[\frac{3}{r} + \frac{1}{r'} - \frac{4 \cos \theta}{\rho} \right] \quad (12)$$

where the notation has been 'generalized' somewhat.

The fixed aberrations of the mirror wavefront must be combined with the grating aberrations and the latter are different for different wavelengths. We have already considered the behavior of the w^2 (focussing) term and from Fig. 2 we recall that the actual r_2' values obtaining are such as to maintain only approximate focus. However, to get a qualitative feeling for the behavior let us suppose for a moment that (2) is exactly satisfied. This makes it possible to follow the behavior of the grating aberrations analytically. The w^2 term now vanishes and the κ^2 (astigmatism) term is given by (using (2) and remembering $r_1' \rightarrow \infty$):

$$C_{02} = \frac{1}{2} \tan^2 \theta_2 \left[\frac{\cos \alpha_2 + \cos \beta_2}{R_2} \right] \quad (13)$$

Firstly we note that $C_{02} = 0$ for $\beta_2 = 0$ i.e. at the Wadsworth wavelength. We also see since $(\cos\alpha_2 + \cos\beta_2)$ is approximately constant and $\tan^2\beta_2$ is always positive that C_{02} is always positive. Thus, the two astigmatism terms are always additive. In other words, both optics introduce into the wavefront a cylindrical curvature of the same sense. For $\lambda = 0$ (13) reduces to the same form as the λ^2 term for the mirror as expected. It is of interest to compare the astigmatism of the grating in the Wadsworth mount with that in the equivalent Rowland Circle mount. Some sample figures, with $\theta=6^\circ$, $1/d=2400\text{gr/mm}$, and a groove length of 160 mm, are:

$\lambda(\text{\AA})$	Full line	Full line
	length (mm)	length (mm)
	Rowland	Wadsworth
0	3.50	1.75
1000	8.26	.04
2000	22.73	3.07

Showing the advantage of the Wadsworth mount for cases where astigmatism is important.

For the coma terms in (7) we note first that, due to the sine factor, the grating coma vanishes at the Wadsworth wavelength. Also, since the sine factor is an odd function of β_2 the coma changes sign at the Wadsworth wavelength and is additive with the mirror coma on one side of λ_w and partially cancelling on the other. Clearly, at $\lambda = 0$ $\beta_2 = -\theta$ and the two coma terms will have the same form and the same sign. Additive coma terms would be expected for this case from sine condition arguments. Therefore, for wavelengths above the Wadsworth wavelength there is partial cancelling of the coma or some straightening of the focal line.

In different language the effect of the grating is to twist the wavefront relative to the Gaussian reference sphere so that it lags on one side and leads on the other. The twist reverses at the Wadsworth wavelength. We can follow this qualitative behavior through the wavelength range by looking at the ray traces (grating only) shown in Fig. 5. The rise and fall of the astigmatism and the change in sign of the coma are clearly evident. The ray traces are exact in the sense that the actual value of r'_2 is used rather than the exact focus value.

6. Source Structure

Thus far, we have considered the effect of a point source and we now turn to more realistic models of the source. For large aperture optics we must consider the effect of the finite arc of the electron trajectory which sends light into the instrument. For the Brookhaven geometry we have an arc of radius 1.91m and length 105mm. Such an arc has a sag of 0.72mm which is not negligible compared to the beam width (2σ) of 1.0mm. So we expect some horizontal broadening. The most important effect is the increase in the vertical emittance of the photon beam which occurs due to the inclusion of photons from sources distributed all along the arc. This is of special importance for instruments using the source as entrance slit because it determines the resolution. If we define an effective source plane perpendicular to the arc and half way along it we can calculate phase space areas representing this source. One could then easily calculate the effect of an imaging system. The calculation of the phase space properties of the effective source, due to a finite arc, has been carried out in detail by Green.⁽¹³⁾ This calculation is quite cumbersome but the most important result is expressed using a function $ef(a,Y)$ defined as

$$ef(a,Y) = \int_0^Y \frac{1}{\cos t} \exp \left[-\frac{1}{2} a^2 \cos^2 t \right] dt \quad (14)$$

where $a = y/\sigma_y$, y being the vertical co-ordinate and σ_y being the e-beam vertical σ . Y is given by

$$\tan Y = \frac{\sigma_s}{\sigma_y}$$

Where σ is the Synchrotron radiation angular σ and s is the half length of the emitting arc. $ef(a,Y)$ is proportional to the differential intensity distribution $F(y)$ or

$$dF(y) = K \frac{dy}{\sigma_y \sqrt{2\pi}} ef(a,Y) \quad (15)$$

K being a constant. Some examples of $ef(a,Y)$ are shown in Fig. 6. We see the general effect, which is that for cases where a large horizontal angle is accepted, there is an overall broadening of the effective source size. The broadening of the full width at half maximum is quite modest but large non-Gaussian tails are produced.

To get a feeling for how the back and front of the source contribute we consider a simpler case as illustration. Consider a line source along the x axis centered on $x = 0$ (see Fig. 7(a)). Suppose this is imaged as shown with lateral magnification M . The width y of the defocussed blur in the focal plane due to the light coming from a point at x is given by

$$y = \frac{M^2 x}{f_n} + y_{ab} \quad (16)$$

Where f_n is the focal ratio and y_{ab} is the width of the aberration blur of the in-focus image of the $x = 0$ point. Let the intensity emitted by the source be q per unit length. Then the light emitted by ' dx ' at x is $q dx$ and this contributes the 'slice' AB in the intensity distribution curve in Fig. 7(b). We thus have $2dI = q dx/y$ so that

$$I(y) = \frac{1}{2} \int_y^{y_{\max}} \frac{q dx}{y}$$

$$\text{From (14) } dx = \frac{f_n dy}{M^2}$$

$$I(y) = \frac{q f_n}{2M^2} \int_y^{y_{\max}} \frac{dy}{y} = \frac{q f_n}{2M^2} \ln \left(\frac{y_{\max}}{y} \right)$$

$$y_{\text{HWHM}} \text{ is now given by } I(y_{\text{HWHM}}) = \frac{1}{2} I(y_{\text{ab}})$$

$$\text{or } \ln \left[\frac{y_{\max}}{y_{\text{HWHM}}} \right] = \frac{1}{2} \ln \left[\frac{y_{\max}}{y_{\text{ab}}} \right]$$

$$\text{Hence } y_{\text{FWHM}} = 2 \sqrt{y_{\max} y_{\text{ab}}} \quad (17)$$

The values of $y_{\max}$ and y_{ab} can be obtained either from (7) and (8) or from ray traces. For the Brookhaven geometry we get $y_{\max} = 0.25\text{mm}$, $y_{\text{ab}} = 0.031\text{mm}$ and $y_{\text{FWHM}} = 0.18\text{mm}$. For a rough calculation of the resolution we could combine this quadratically with the quoted electron beam width (2 σ) of 0.2mm to get an effective 'entrance slit' size of 0.27mm. A similar result is obtained by use of Fig. 6.

7. Calculation of the Resolution

The primary determinant of the resolution is the effective size of the source through the relationship:

$$\Delta \lambda_s = \frac{h d \cos \alpha}{r_1} \quad (18)$$

Where $\Delta \lambda_s$ is the source size limit of wavelength resolution, h is the source size and r_1 the source/mirror distance. For $1/d = 2400\text{gr/mm}$ $\Delta \lambda_s = 0.39\text{\AA}$. For $1/d = 1200\text{gr/mm}$, $\Delta \lambda_s = 0.79\text{\AA}$ and for $1/d = 3600\text{gr/mm}$, $\Delta \lambda_s = 0.26\text{\AA}$. One can calculate the broadening due to the defocus expressed in

Fig. 2 and this has no effect within 10% except for a small part of the range at the very longest wavelengths where it is slightly more than 10%. Other aberrations are mostly small. The effect of coma is negligible for a large range either side of the Wadsworth wavelength. For example it gives less than 0.1 μ broadening from 400 μ to 1400 μ ($1/d = 2400\text{gr/mm}$). At 400 μ the comatic curvature contributes 0.09 μ or .04mm broadening. Adding this to the .061mm from the mirror we still have only 0.23 μ which is not yet a major problem. At the long wavelength end at 2000 μ (say) the coma contribution from the grating is 0.21 μ but this is to be combined with -0.13 μ from the mirror, again producing a negligible effect.

The overall conclusion is that the resolution is given with good accuracy by the source size limit provided we use the effective source size that includes the broadening due to the depth of the source. This latter is the only significant effect worsening the geometrical resolution and we can note that it would not be eliminated by using a parabolic mirror. Only a 'magic' mirror⁽¹⁴⁾ would make any difference.

As to the horizontal width of the image, we must consider the total source width including the curvature of the electron beam (1.72mm) and the astigmatism of the concave mirror, which gives a FWHM of 2.50mm. Adding these quadratically gives 3.0mm. This is larger than the grating contribution over the entire range and apart from around 2000 μ it is much larger. We thus adopt as our working value of the image size 3.0mm (H) x 0.19mm (V).

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Figure Captions

- Figure 1. Geometrical layout of various possible monochromator arrangements. The scale has been distorted for clarity.
- Figure 2. Focal curve for the Brookhaven monochromator.
- Figure 3. Notation and co-ordinate system for optical path function analysis.
- Figure 4. Ray trace for the mirror in parallel light $AB = 24\text{mm}$, $BD = 158\text{mm}$. The focal line of length 1.8mm has an overall curve as seen due to sagittal coma. The spots in the grid ABCD are the ray intersections with the mirror. Note the small curved line produced by the five spots along AB and CD. This is produced by a higher order aberration (C_{22}) than those considered in this paper.
- Figure 5. Ray traces for the spherical grating in parallel light. The number under each pattern is the wavelength in Å. The pattern of ray intersections is the same as for figure. 4. Each pattern is for the actual distance of the grating from the exit slit using the focussing correction shown in figure 2. We can thus discern the effect of the three main aberrations: (i) The wavelengths 600Å and 1600Å shown by figure 2 to be in focus are indeed in focus. (ii) The astigmatism decreases going up to the Wadsworth wavelength (866Å) and then increases again. (iii) The comatic curvature changes sign at the Wadsworth wavelength.
- Figure 6. The function $ef(a,Y)$ as calculated by Green¹³ and explained in the text. Curves 1 through 6 are for Y values 0.1, 0.5, 1.0, 1.2, 1.4 and 1.5 respectively.
- Figure 7. (a) Schematic showing a light source extended along the direction of emission. The light is focussed to a focal plane, the light from the extreme end producing the defocussed blur of width y_{max} (b) Typical intensity distribution. Light from x that gives a blur of height y in the focal plane contributes the 'slice' AB. The intensity for any particular y value includes contributions from 'slices' of width y and greater.

$$SM + MG = GS'$$

(a) FOLDED McPHERSON

$$SM + MG \sim 3GS'$$

(b) POUÉY TYPE UNSYMMETRICAL MOUNT

SM, MG, GS': NO FIXED RELATIONSHIP

(c) MODIFIED WADSWORTH

SM, MG, GS' RELATIONSHIP DETERMINED BY CHOICE
OF WAVELENGTH OF ABERRATION CANCELLING

(d) MONK-GILLIESON

Fig. 1.

FIG. 2.

Fig. 3.

Fig. 4.

Fig. 5.

Fig. 6.

Fig. 7.