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IMAGE FORMATION IN A MIYAKE MONOCHROMATOR USED IN DIVERGENT LIGHT

by

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1. INTRODUCTION

Several monochromators have in recent years been constructed based on the geometry originally given by Miyake[1,2,3]. This consists of a plane grating and a spherical focusing mirror in a constant deviation geometry. The assumption was made in the original designs that the light source was far enough away so that the light could be considered to be parallel. The purpose of this paper is to consider the action of the plane grating and spherical mirror when situated relatively near the source point so that the light has to be considered to be divergent.

2. THE MONOCHROMATOR IN PARALLEL LIGHT

Figure 1 gives the monochromator geometry. It can be seen that the mirror and exit slit both occupy fixed horizontal positions in relation to the grating and that the wavelength is scanned by simple rotation of the grating. This arrangement satisfies the requirement for constant deviation which can be expressed as,

$$\alpha - \beta = 2\theta = \text{constant.} \qquad (1)$$

Note: β is − ve when on the opposite side of the normal to α, i.e. as in this case. α and β are the angles of incidence and diffraction respectively.

It can be seen that the paraxial focusing equation becomes,

$$\frac{1}{\infty} + \frac{1}{x} = \frac{2}{R\cos\theta}\,; \qquad x = \frac{R}{2}\cos\theta \qquad (2)$$

where θ is the angle of incidence for the mirror, R is the radius of the mirror and x is the mirror to slit distance. The horizontal distance between the grating and mirror has to satisfy the geometrical relation given by

$$y' = x\cot 2\theta \qquad (3)$$

where y' is the horizontal distance between the grating and mirror and x is the vertical distance between the grating and mirror. As the horizontal distance between the grating and slit is the sum of y' and x we have

$$y = \frac{R}{2}\cos\theta + x\cot 2\theta \qquad (4)$$

In practice y, x and R are fixed and θ is a variable. Equation (4) has two solutions for θ and hence from eq. (2) two corresponding mirror slit distances. The mirror is therefore movable along a horizontal line level with the exit slit so that one or other of the two focal positions can be used. For a single mirror, this type of monochromator therefore has two zero order positions. By a correct choice of y, x and R, West[2] showed that the zero order angle can be arranged so the higher order suppression by selective reflection can be usefully employed.

The resolution limit imposed by the vertical source size can be obtained from the grating equation.

$$Nk\lambda = \sin\alpha + \sin\beta$$

$$\frac{d\lambda}{d\alpha} = \frac{1}{Nk}\cos\alpha \qquad (\beta \text{ const}) \qquad (5)$$

where N is the grating groove density and k is the order of diffraction.

$$d\alpha = S/L$$

where S is the vertical source height and L is the source to grating distance.

$$\therefore\ d\lambda = \frac{1}{Nk}\,\frac{S}{L}\cos\alpha \qquad (6)$$

The angular dispersion can similarly be obtained from the grating equation,

$$\frac{d\lambda}{d\beta} = \frac{1}{Nk}\cos\beta \qquad (\alpha \text{ const}) \qquad (7)$$

The linear dispersion in the focal plane is then obtained from the angular dispersion by making the assumption,

$$d\beta = \frac{dy}{x} \qquad (8)$$

where dy is a distance in the dispersive direction. The implications of this assumption will be examined later. This leads to a relation for the linear dispersion.

$$\frac{d\lambda}{dy} = \frac{1}{Nkx}\cos\beta \qquad (9)$$

The resolution of this type of monochromator was recognised not only to be limited by the vertical source size but also by spherical aberration and coma associated with the focusing spherical mirror. This was limited by restriction of the vertical aperture to small values (e.g. ref.2, West; 0.05 mrad).

3. THE MONOCHROMATOR IN DIVERGENT LIGHT

With the advent of high brightness storage rings with small vertical source sizes it is now no longer necessary to place entrance slitless monochromators as far away from the source point to achieve good source limited resolution. It therefore becomes necessary to re-examine the focusing and dispersion properties for the case of non-parallel light.

3.1 Focusing

The general arrangement is given in fig.2. The action of the plane grating in divergent light has been analysed by Murty[6] by examining the focusing term in the optical path function for a spherical grating with the radius set to infinity. The focusing term is given by

$$C_{20} = \frac{1}{2}\left[\left(\frac{\cos^2\alpha}{L} - \frac{\cos\alpha}{R}\right) + \left(\frac{\cos^2\beta}{L'} - \frac{\cos\beta}{R}\right)\right] \qquad (10)$$

where L is the object distance and L' is the image distance. The radius is set to infinity and by setting C_{20} to zero we can find the position of the monochromatic source point.

$$L' = -L\,\frac{\cos^2\beta}{\cos^2\alpha} \qquad (11)$$

Figure 3 shows the action of the grating in divergent light. The negative sign implies that the focus is behind the grating and acts as the virtual source point for following focusing optics. Clearly from eq. (11) the virtual source distance is a strong function of wavelength.

To characterise the image formed by a fixed spherical mirror of a wavelength dependent source we must obtain the virtual source size and divergence. Figure 4 gives the geometry for calculating the virtual source divergence.

$$T = OB\cos\beta$$
$$\phi' = T/L'$$
$$OB = AO\sin\phi/\sin\angle ABO$$
$$\sin\angle ABO \simeq \cos\alpha;\ AO = L$$
$$\therefore T = L\phi\cos\beta/\cos\alpha;\ L' = -L\cos^2\beta/\cos^2\alpha$$
$$\therefore \phi' = -\phi\cos\alpha/\cos\beta \qquad (12)$$

Figure 5 gives the geometry for calculation of the virtual source magnification. It can be seen directly that

$$S' = AO\cos\beta;\quad AO = S/\cos\alpha$$

$$\therefore S' = S\cos\beta/\cos\alpha \qquad (13)$$

We can now derive an expression for the demagnification of the monochromator. Figure 6 shows the geometry used.

$$I = S'\,\frac{F}{(P - L')} \qquad (14)$$

where I is the monochromatic image size at the focal plane given by F.

P is the distance between the grating and mirror.

Substitute for S' from (13)

$$I = S \frac{\cos\beta}{\cos\alpha} \frac{F}{(P - L')} \qquad (15)$$

substitute for L' from (11)

$$I = S \frac{\cos\beta}{\cos\alpha} \frac{F}{\left[\frac{L \cos^2\beta}{\cos^2\alpha} + P\right]} \qquad (16)$$

$$\text{let } \omega = \cos\beta/\cos\alpha \qquad (17)$$

$$I = S \frac{F}{L\omega + P/\omega} \qquad (18)$$

Equation 16 gives the overall monochromatic magnification of the source. It can be seen that if P is small relative to L' then

$$I = S \frac{F}{L} \frac{\cos\alpha}{\cos\beta}$$

This is the expression for magnification in a single element diffracting and focusing device. The magnification expression contains the term F for the monochromatic focal length. Clearly, as the virtual object distance is a function of wavelength the image distance also will be a function of wavelength. Using the paraxial focusing equation we have,

$$\frac{1}{(P - L')} + \frac{1}{F} = \frac{2}{R \cos\theta} \text{ ; let } R' = R \cos\theta \qquad (19)$$

$$\frac{1}{F} = \frac{2}{R'} - \frac{1}{(P - L')} \qquad (20)$$

$$F = \frac{R'(P - L')}{2(P - L') - R'} \qquad (21)$$

We can now substitute the monochromatic focal length F into (15). For the full expression of the magnification

$$I = S \frac{\cos\beta}{\cos\alpha} \frac{R'}{[2(P - L') - R']} \qquad (22)$$

In practice therefore the exit slits would be moved along the beamline so that they would always coincide with the monochromatic focal point.

3.1 Dispersion

The geometry for calculation of the dispersion is given in fig.7. The angular dispersion is obtained directly from the grating equation,

$$\frac{d\lambda}{d\beta} = \frac{1}{Nk} \cos\beta \qquad (23)$$

To obtain the linear dispersion $d\lambda/dy$ we need to find the relationship of $d\beta$ to dy where dy is a linear distance at the monocromatic focal point in the plane of dispersion.

From fig.7 it can be seen that the dispersion can be calculated by considering the centre of the grating as a virtual source for the central rays. By using the paraxial ray equation we can calculate the intersection point and the displacement in the focal plane.

$$\frac{1}{P} + \frac{1}{m} = \frac{2}{R'}$$

$$m = \frac{PR'}{2P - R'} \qquad (24)$$

If the angle at the crossing point is Φ and the distance from the crossing point to the focal plane is B',

$$dy = \Phi B' \qquad (25)$$

$$B' = \left|F - m\right| \text{ ; } \Phi = d\beta\, P/m \qquad (26)$$

$$\therefore d\beta = dy \frac{m}{P} \frac{1}{\left|F - m\right|} \qquad (27)$$

Substituting (27) into (23) gives

$$\frac{d\lambda}{dy} = \frac{1}{Nk}\cos\beta\,\frac{m}{P}\,\frac{1}{\left|F - m\right|} \qquad (28)$$

Substituting (24) into (28) and rearranging

$$\frac{d\lambda}{dy} = \frac{1}{Nk}\cos\beta\,\frac{1}{\frac{2PF}{R'} - F - P} \qquad (29)$$

We now have to substitute back in for R' in terms of L' + P and F from (19) and rearrange.

$$\frac{d\lambda}{dy} = \frac{1}{Nk}\cos\beta\,\frac{(P/L - 1)}{F} \qquad (30)$$

We can now substitute for F from (19).

$$\frac{d\lambda}{dy} = \frac{1}{Nk}\cos\beta\,\frac{1}{L'}\left[\frac{2(P/L)}{R'} - 1\right] \qquad (31)$$

This expression is therefore the full expression for the linear dispersion. The slits as before have to track the focal point as a function of wavelength in accordance with eq. (21).

Equation (30) can now be compared with the generally used 'standard' form of dispersion given by eq. (9)

$$\frac{d\lambda}{d\beta} = \frac{1}{Nk}\cos\beta\,\frac{1}{x}$$

This form can now be seen to be an approximation in two ways. Firstly, the mirror to slit distance is given as a constant (x) which results from the assumption of parallel light and secondly the finite separation of the dispersing and focusing element is ignored. The separation clearly gives the P/FL term in eq. (30) which of course vanishes as the grating and mirror converge.

4. SOURCE LIMITED RESOLUTION

We have obtained expressions for the magnification and the dispersion. From these we can therefore find the source limited resolution which should correspond to the simple form given in eq. (6) which was obtained directly from the grating equation

$$d\lambda = \frac{1}{Nk}\,\frac{S}{L}\cos\alpha$$

We have obtained expressions for dλ/dy and for I. dy and I have the same meaning in this case so by substituting in eq. (30) for dy given in eq. (15) we have

$$d\lambda = \frac{1}{Nk}\cos\beta\left(\frac{P - L'}{L'F}\right) S\,\frac{\cos\beta}{\cos\alpha}\,\frac{F}{(P - L')}$$

Substituting for L' from (11) we have,

$$d\lambda = \frac{1}{Nk}\cos\beta\left(\frac{\cos^2\alpha}{L\cos^2\beta}\right) S\,\frac{\cos\beta}{\cos\alpha}$$

$$d\lambda = \frac{1}{Nk}\,\frac{S}{L}\cos\alpha$$

As expected therefore the same simple form of the grating equation has been derived using the correct expressions for the magnification and dispersion.

5. DEFOCUS

The analysis so far has assumed that the exit slits are tracked so that they stay coincident with the monochromatic image distance given by eq. (21). If the slits are fixed relative to the grating then the effect is that the monochromator is in focus only at one wavelength. This wavelength may be chosen by selection of the appropriate values for R and θ. If the slits are not at the monochromatic focal point then the resolution is degraded by an amount proportional to the separation of the focus and the slits. It can be seen from eq. (11) that in negative order the monochromatic virtual source moves towards the grating and in positive order away from the grating. From an examination of the focus eq. (21) it can be seen that the movement of the image will therefore be much more severe in negative order than in positive order. If the slits are fixed therefore the defocus contribution to the resolution can be limited by choosing a wavelength in the middle of the range to be in focus and by operating in positive order. In the normal Miyake calculated for parallel light, the monochromator will only be in focus at zero wavelength; i.e. zero order. A further way to control defocus is to select a new zero order angle for each wavelength. In this way, the monochromator will always be in focus but necessitates moving the mirror with respect to the slits for each wavelength.

From fig.1 it can be seen that,

$$x = y - y'$$

$$\therefore \ell b = x = y - x/\tan 2\theta$$

where ℓb is the image distance.

Let $R' = R\cos\theta$ as before and we can find an expression for the object distance as a function of ℓb and R'.

$$\frac{1}{\ell a} + \frac{1}{\ell b} = \frac{2}{R'}$$

$$\ell a = \frac{R'\,\ell b}{2\ell b - R'} \qquad (32)$$

The object distance defined by the sum of the virtual source distance and the separation of the grating and mirror therefore has to match that defined by the geometry given in eq.(32)

$$\ell a = P - L' = x/\sin 2\theta - L' \qquad (33)$$

Combination of (33) and (32) therefore yields an expression for the virtual source point as a function of θ

$$-L' = \frac{R'\,\ell b}{2\ell b - R'} - \frac{x}{\sin 2\theta} \qquad (34)$$

$$\text{where } \ell b = y - x\cot 2\theta \qquad (35)$$

The virtual source point given by the grating can always be made to give that required by the focusing optics as from eq. (11) we can see that L' can go from zero at the negative order horizon to infinity at the positive order horizon.

$$L' = -L\,\frac{\cos^2\beta}{\cos^2\alpha} \qquad \ldots\ldots (11)$$

Equations (34) and (11) can now be combined and solved for λ

$$\frac{\cos^2\beta}{\cos^2\alpha} = \frac{1}{L}\left(\frac{R'\ell b}{2\ell b - R'} - \frac{x}{\sin 2\theta}\right)$$

$$\text{let } G = \left(\frac{1}{L}\left(\frac{R'\,\ell b}{2\ell b - R'} - \frac{x}{\sin 2\theta}\right)\right)^{1/2} \qquad (36)$$

$$\frac{\cos^2\beta}{\cos^2\alpha} = G^2\;;\; \cos\beta - G\cos\alpha = 0$$

if we define the angle turned from zero order to be ϕ then

$$\alpha = \phi + \theta\;;\; \beta = \phi - \theta$$

$$\cos(\phi - \theta) - G\cos(\phi + \theta) = 0$$

expanding cos and rearranging we have

$$\cos\phi\,\cos\theta(1 - G) + \sin\phi\,\sin\theta(1 + G) = 0 \qquad (37)$$

$$\text{let } H = \cos\theta(1 - G);\; J = \sin\theta(1 + G) \qquad (38)$$

substituting (38) in (37) we have

$$\cos\phi = \frac{-J}{H}\sin\phi$$

which can be expressed as

$$\sin\phi = \frac{-H}{(H^2 + J^2)^{1/2}} \tag{39}$$

By rearranging the grating equation we can exprees the wavelength only as a function of the turning angle ϕ.

$$Nk\lambda = 2\cos\theta\,\sin\phi \tag{40}$$

Substituting (40) into (39) yielde

$$\lambda = \frac{2}{Nk}\cos\theta\,\frac{H}{(H^2 + J^2)^{1/2}} \tag{41}$$

This equation expresses the in focus wavelength as a function of θ. To operate in this mode would require altering the mirror angle θ as well as the mirror slit distance for each wavelenth.

The most practical eolution would be to move the slite along the bsamline as a function of wavelength. In this way the monochromator would always be in focus and so the resolution would only be limited by the source height and coma produced by the spherical focusing mirror. This coma could be reduced by operating at low demagnification. This would require a large image distance which would give a large dispereion. This would make optical alignment much easier due to the large source limit exit slit openings.

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FIGURE CAPTIONS

Fig. 1 Geometry of a Miyake monochromator.

Fig. 2 Constant deviation plane grating monochromator.

Fig. 3 Plane grating in divergent light.

Fig. 4 Angular divergence of virtual source.

Fig. 5 Magnification of virtual source.

Fig. 6 Image formation in the PGM.

Fig. 7 Calculation of dispersion for separated diffraction and focusing condition.

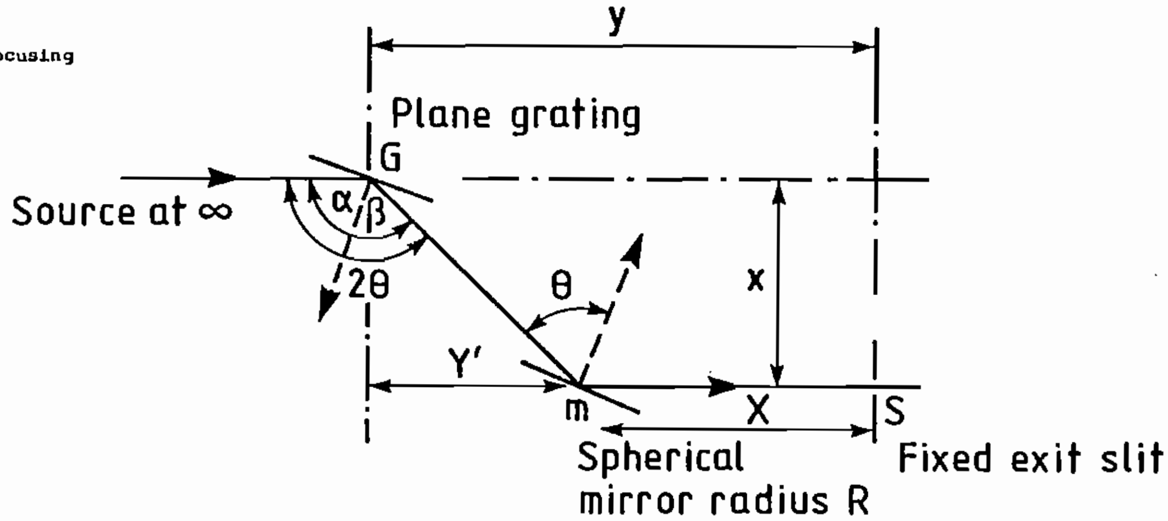


Fig. 1

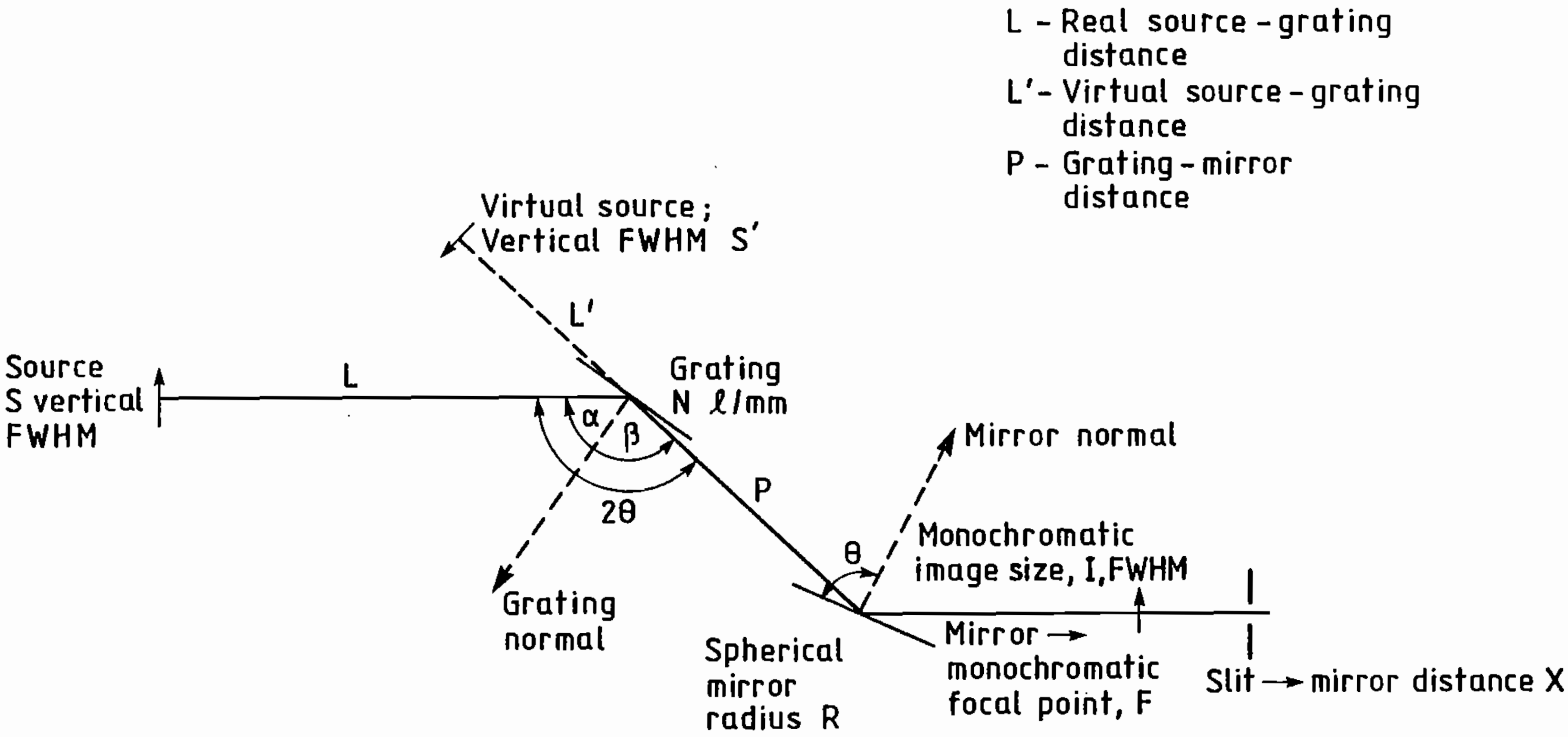
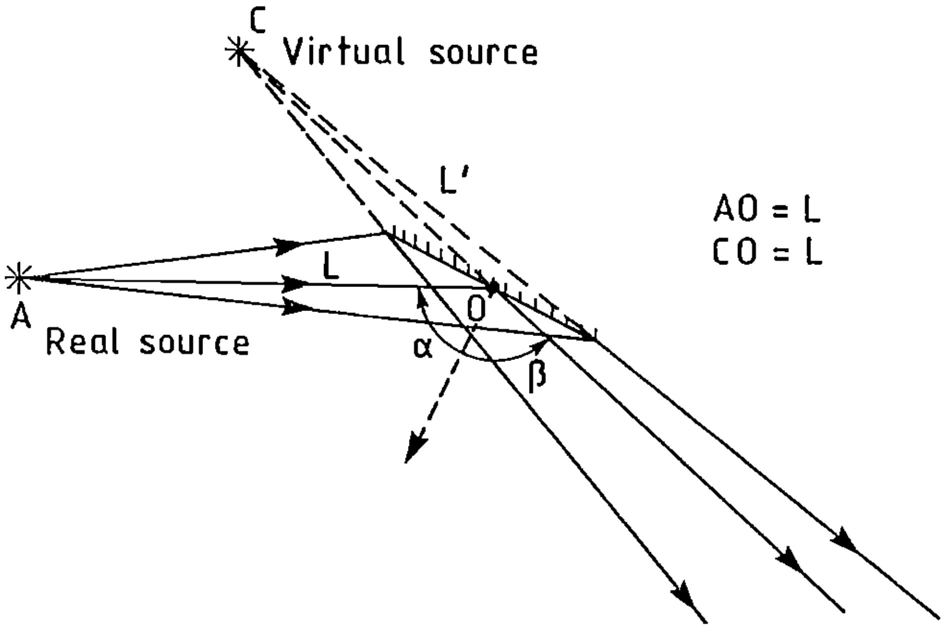
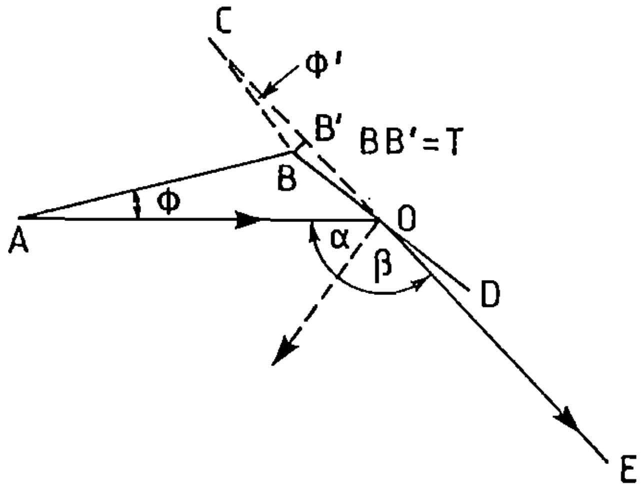

L - Real source - grating distance
L'- Virtual source - grating distance
P - Grating - mirror distance
Virtual source ; Vertical FWHM S'
L'
Source S vertical FWHM
L
Grating N ℓ/mm
α
β
2θ
P
Mirror normal
Monochromatic image size, I, FWHM
θ
Grating normal
Spherical mirror radius R
Mirror → monochromatic focal point, F
Slit → mirror distance X

Fig. 2



C
Virtual source
L'
AO = L
CO = L
L
A
Real source
O
α
β

Fig. 3



C
Φ'
B'
BB'=T
B
Φ
A
O
α
β
D
E

Fig. 4

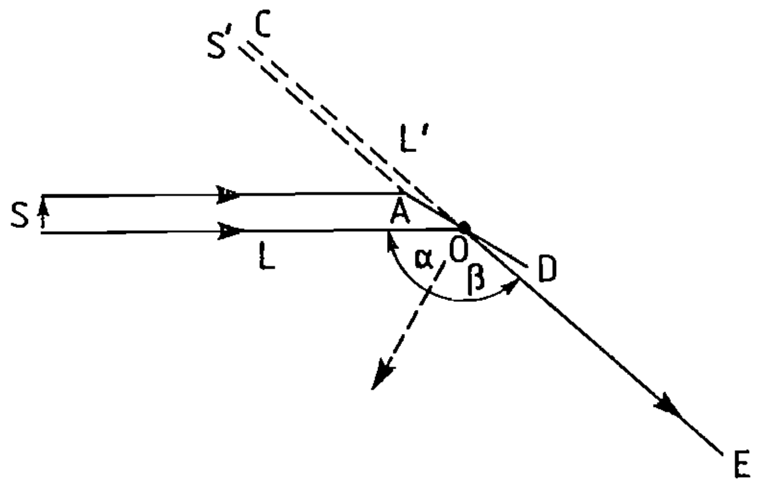


Fig. 5

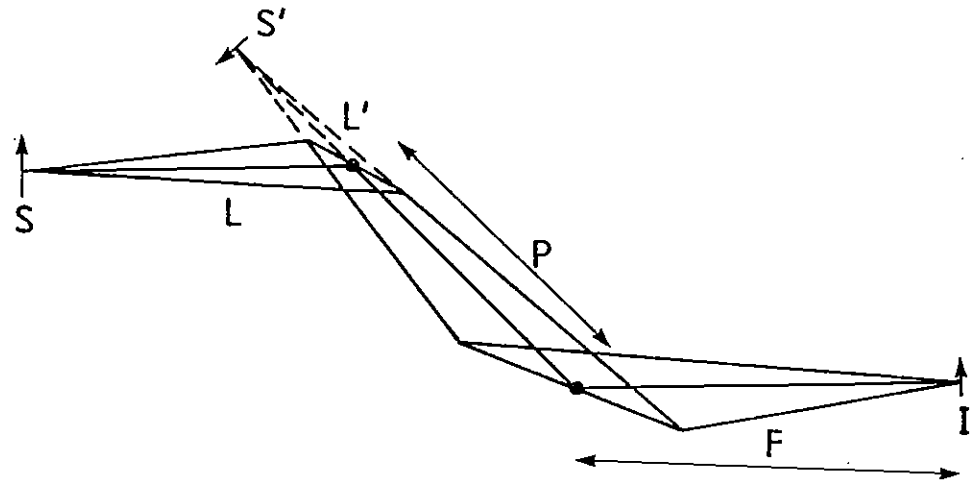


Fig. 6

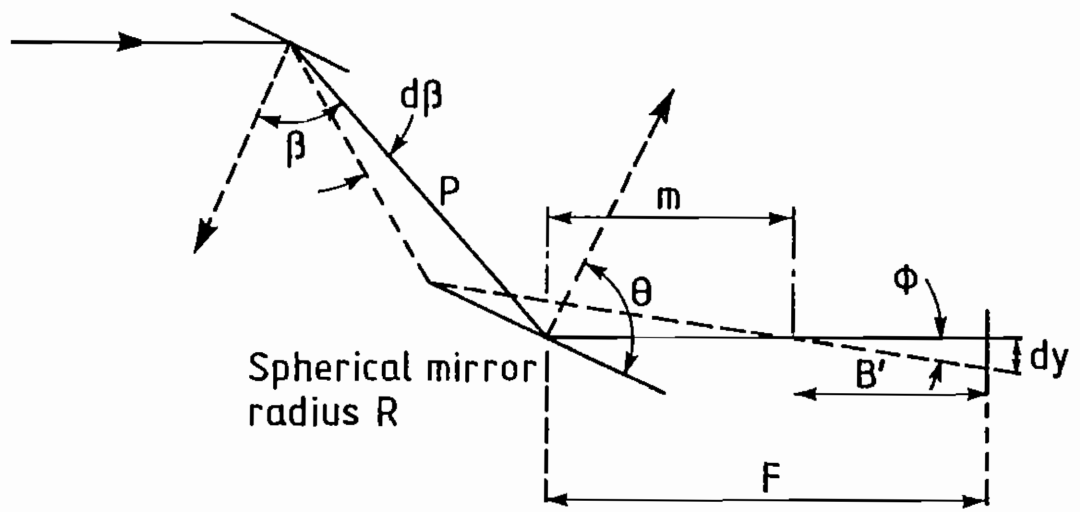


Fig. 7