Section 4.3 GRATINGS AND MONOCHROMATORS

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A. DIFFRACTION PROPERTIES

A.1 Notation and sign convention

We adopt the notation of Fig. 4-6, in which a and b have opposite signs if they are on opposite sides of the normal.

A.2 Grating equation

The grating equation may be written

$$m l = d_0(\sin a + \sin b) \quad . \tag{1}$$

The angles a and b are both arbitrary, so it is possible to impose various conditions relating them. If this is done, then for each l, there will be a unique a and b. The following conditions are used:

(i) On-blaze condition:

$$\alpha + \beta = 2\theta_B \quad , \tag{2}$$

where q_B is the blaze angle (the angle of the sawtooth). The grating equation is then

$$m\lambda = 2d_0 \sin \theta_B \cos(\beta + \theta_B) \quad . \tag{3}$$

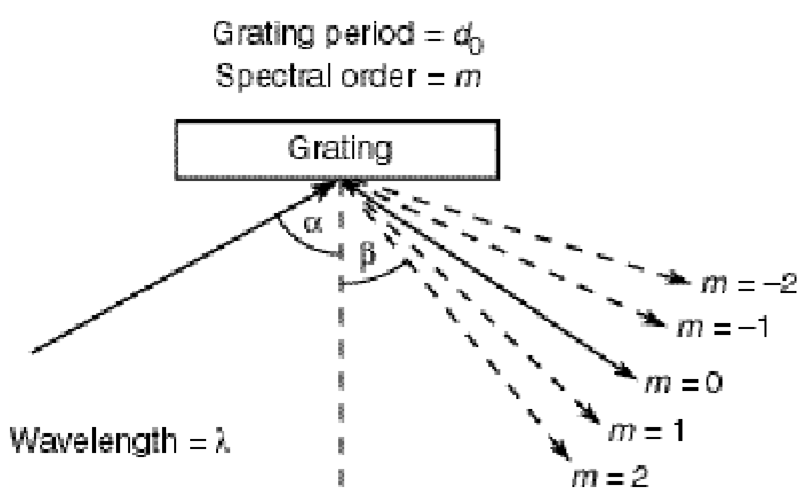

Fig. 4-6. *Grating equation notation.*

(ii) Fixed in and out directions:

$$\alpha - \beta = 2\theta \quad , \tag{4}$$

where $2q$ is the (constant) included angle. The grating equation is then

$$m\lambda = 2d_0 \cos\theta \sin(\theta + \beta) \quad . \tag{5}$$

In this case, the wavelength scan ends when a or b reaches 90°, which occurs at the horizon wavelength $l_H = 2d_0 \cos^2 q$.

(iii) Constant incidence angle: Equation (1) gives b directly.

(iv) Constant focal distance (of a plane grating):

$$\frac{\cos\beta}{\cos\alpha} = \text{ a constant } c_{ff} \quad , \tag{6}$$

leading to a grating equation

$$1 - \left(\frac{m\lambda}{d} - \sin\beta\right)^2 = \frac{\cos^2\beta}{c_{ff}^2} \quad . \tag{7}$$

Equations (3), (5), and (7) give b (and thence a) for any l. Examples of the above a-b relationships are (for references see http://www-cxro.lbl.gov/):

(i) Kunz et al. plane-grating monochromator (PGM), Hunter et al. double PGM, collimated-light SX700 PGM

(ii) Toroidal-grating monochromators (TGMs), spherical-grating monochromators (SGMs, "Dragon" system), Seya-Namioka, most aberration-reduced holographic SGMs, variable-angle SGM, PGMs

(iii) Spectrographs, "Grasshopper" monochromator

(iv) Standard SX700 PGM and most variants

B. FOCUSING PROPERTIES

The study of diffraction gratings (for references see http://www-cxro.lbl.gov/) goes back more than a century and has included plane, spherical [1], toroidal, and ellipsoidal surfaces and groove patterns made by classical ("Rowland") ruling [2], holography [3,4], and variably spaced ruling [5,6]. In recent years the optical design possibilities of holographic groove patterns and variably spaced rulings have been extensively developed. Following normal practice, we provide an analysis of the imaging properties of gratings by means of the path function F [7]. For this purpose we use the notation of Fig. 4-7, in which the zeroth groove (of width d_0) passes through the grating pole O, while the nth groove passes through the variable point P(ξ,w,l). The holographic groove pattern is taken to be made using two coherent point sources C and D with cylindrical polar coordinates (r_C,g,z_C), (r_D,d,z_D) relative to O. The lower (upper) sign in Eq. (9) refers to C and D both real or both virtual (one real and one virtual), for which case the equiphase surfaces are confocal hyperboloids (ellipses) of revolution about

CD. Gratings with varied line spacing $d(w)$ are assumed to be ruled according to $d(w) = d_0(1 + v_1 w + v_2 w^2 + ...)$.

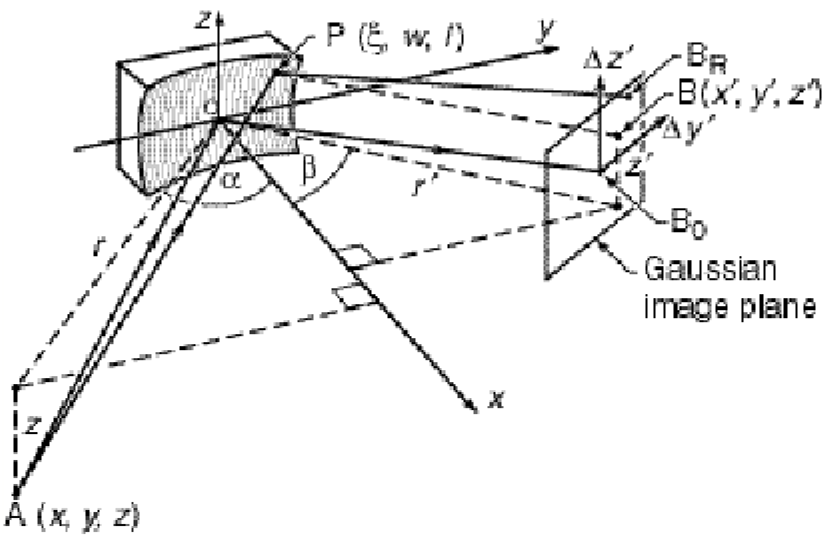

Fig. 4-7. *Focusing properties notation.*

We consider all the gratings to be ruled on the general surface

$$x = \sum_{ij} a_{ij} w^i l^j$$

and the a_{ij} coefficients are given below.

Ellipse coefficients a_{ij}

$$a_{20} = \frac{\cos\theta}{4}\left(\frac{1}{r} + \frac{1}{r'}\right) \qquad a_{12} = \frac{a_{20} A}{\cos^2\theta}$$

$$a_{30} = a_{20} A \qquad a_{22} = \frac{a_{20}\left(2A^2 + C\right)}{2\cos^2\theta}$$

$$a_{40} = \frac{a_{20}\left(4A^2 + C\right)}{4} \qquad a_{04} = \frac{a_{20} C}{8\cos^2\theta}$$

$$a_{02} = \frac{a_{20}}{\cos^2\theta}$$

The other a_{ij}'s with $i + j \leq 4$ are zero. In the expressions above, r, r', and q are the object distance, image distance, and incidence angle to the normal, respectively, and

$$A = \frac{\sin\theta}{2}\left(\frac{1}{r} - \frac{1}{r'}\right) \quad , \quad C = A^2 + \frac{1}{rr'} \quad .$$

Toroid coefficients a_{ij}

$$a_{20} = \frac{1}{2R} \qquad a_{22} = \frac{1}{4\rho R^2}$$

$$a_{40} = \frac{1}{8R^3} \qquad a_{04} = \frac{1}{8\rho^3}$$

$$a_{02} = \frac{1}{2\rho}$$

Other a_{ij}'s with $i + j \leq 4$ are zero. Here, R and r are the major and minor radii of the bicycle-tire toroid.

The a_{ij}'s for spheres; circular, parabolic, and hyperbolic cylinders; paraboloids; and hyperboloids can also be obtained from the values above by suitable choices of the input parameters r, r', and q.

Values for the ellipse and toroid coefficients are given to sixth order at http://www-cxro.lbl.gov/.

B.1 Calculation of the path function *F*

F is expressed as

$$F = \sum_{ijk} F_{ijk}\, w^i l^j \quad , \tag{8}$$

where

$$F_{ijk} = z^k C_{ijk}(\alpha, r) + z'^k C_{ijk}(\beta, r') + \frac{m\lambda}{d_0} f_{ijk}$$

and the f_{ijk} term, originating from the groove pattern, is given by one of the following expressions:

$$f_{ijk} = \begin{cases} 1 \text{ when } ijk = 100, \ 0 \text{ otherwise} & \text{Rowland} \\ \dfrac{d_0}{\lambda_0}\left[z_C^k C_{ijk}(\gamma, r_C) \pm z_D^k C_{ijk}(\delta, r_D)\right] & \text{holographic} \\ n_{ijk} & \text{varied line spacing} \end{cases} \tag{9}$$

The coefficient F_{ijk} is related to the strength of the i,j aberration of the wavefront diffracted by the grating. The coefficients C_{ijk} and n_{ijk} are given below, where the following notation is used:

$$T = T(r, \alpha) = \frac{\cos^2\alpha}{r} - 2a_{20}\cos\alpha \tag{10a}$$

and

$$S = S(r, \alpha) = \frac{1}{r} - 2a_{02}\cos\alpha \quad . \tag{10b}$$

Coefficients C_{ijk} of the expansion of F

$$C_{011} = -\frac{1}{r} \qquad C_{020} = \frac{S}{2} \qquad C_{022} = -\frac{S}{4r^2} - \frac{1}{2r^3}$$

$$C_{031} = \frac{S}{2r^2} \qquad C_{040} = \frac{4a_{02}^2 - S^2}{8r} - a_{04}\cos\alpha$$

$$C_{100} = -\sin\alpha \qquad C_{102} = \frac{\sin\alpha}{2r^2}$$

$$C_{111} = -\frac{\sin\alpha}{r^2} \qquad C_{120} = \frac{S\sin\alpha}{2r} - a_{12}\cos\alpha$$

$$C_{200} = \frac{T}{2} \qquad C_{202} = -\frac{T}{4r^2} + \frac{\sin^2\alpha}{2r^3}$$

$$C_{211} = \frac{T}{2r^2} - \frac{\sin^2\alpha}{r^3} \qquad C_{300} = -a_{30}\cos\alpha + \frac{T\sin\alpha}{2r}$$

$$C_{220} = -a_{22}\cos\alpha + \frac{1}{4r}\left(4a_{20}a_{02} - TS - 2a_{12}\sin 2\alpha\right) + \frac{S\sin^2\alpha}{2r^2}$$

$$C_{400} = -a_{40}\cos\alpha + \frac{1}{8r}\left(4a_{20}^2 - T^2 - 4a_{30}\sin 2\alpha\right) + \frac{T\sin^2\alpha}{2r^2}$$

The coefficients for which $i \le 4$, $j \le 4$, $k \le 2$, $i + j + k \le 4$, $j + k$ = even are included here.

Coefficients n_{ijk} of the expansion of F

$$n_{ijk} = 0 \quad \text{for} \quad j, k \neq 0$$

$$n_{100} = 1 \qquad n_{300} = \frac{v_1^2 - v_2}{3}$$

$$n_{200} = \frac{-v_1}{2} \qquad n_{400} = \frac{-v_1^3 + 2v_1v_2 - v_3}{4}$$

Values for C_{ijk} and n_{ijk} are given to sixth order at http://www-cxro.lbl.gov/.

B.2 Determination of the Gaussian image point

By definition the principal ray AOB_0 arrives at the Gaussian image point $B_0(r_0', \beta_0, z_0')$ in Fig. 4-7. Its direction is given by Fermat's principal, which implies $[\P F/\P w]_{w=0,l=0} = 0$ and $[\P F/\P l]_{w=0,l=0} = 0$, from which

$$\frac{m\lambda}{d_0} = \sin\alpha + \sin\beta_0 \tag{11a}$$

and

$$\frac{z}{r} + \frac{z_0'}{r_0'} = 0 \quad , \tag{11b}$$

which are the grating equation and the law of magnification in the vertical direction. The tangential focal distance r_0' is obtained by setting the focusing term F_{200} equal to zero and is given by

$$T(r,\alpha) + T(r_0', \beta_0) = \begin{cases} 0 & \text{Rowland} \\ -\dfrac{m\lambda}{\lambda_0}[T(r_C,\gamma) \pm T(r_D,\delta)] & \text{holographic} \\ \dfrac{v_1 m\lambda}{d_0} & \text{varied line spacing} \end{cases} \tag{12}$$

Equations (11) and (12) determine the Gaussian image point B_0 and, in combination with the sagittal focusing condition ($F_{020} = 0$), describe the focusing properties of grating systems under the paraxial approximation. For a Rowland spherical grating the focusing condition, Eq. (12), is

$$\left(\frac{\cos^2\alpha}{r} - \frac{\cos\alpha}{R}\right) + \left(\frac{\cos^2\beta}{r_0'} - \frac{\cos\beta}{R}\right) = 0 \quad , \tag{13}$$

which has important special cases: (i) plane grating, $R = \infty$,
implying

$$r_0' = -r\cos^2 a/\cos^2 b = -r/c_{ff}^2$$

so that the focal distance and magnification are fixed if c_{ff} is held constant; (ii) object and image on the Rowland circle, i.e., $r = R\cos\alpha$, $r_0' = R\cos\beta$, $M = 1$; and (iii) $b = 90°$ (Wadsworth condition). The focal distances of TGMs and SGMs, with or without moving slits, are also determined using Eq. (13).

B.3 Calculation of ray aberrations

In an aberrated system, the outgoing ray will arrive at the Gaussian image plane at a point B_R displaced from the Gaussian image point B_0 by the ray aberrations $\Delta y'$ and $\Delta z'$ (Fig. 4-7). The latter are given by

$$\Delta y' = \frac{r_0'}{\cos\beta_0}\frac{\partial F}{\partial w} \quad , \quad \Delta z' = r_0'\frac{\partial F}{\partial l} \quad , \tag{14}$$

where F is to be evaluated for A = (r,a,z) and B = (r_0', β_0, z_0'). By means of the expansion of F, these equations allow the ray aberrations to be calculated separately for each aberration type:

$$\Delta y_{ijk}' = \frac{r_0'}{\cos\beta_0} F_{ijk} i w^{i-1} l^j \;, \; \Delta z_{ijk}' = r_0' F_{ijk} w^i j l^{j-1} \quad . \tag{15}$$

Moreover, provided the aberrations are not too large, they are additive, so that they may either reinforce or cancel.

C. DISPERSION PROPERTIES

Dispersion properties can be summarized by the following relations.

(i) Angular dispersion:

$$\left(\frac{\partial\lambda}{\partial\beta}\right)_{\alpha} = \frac{d\cos\beta}{m} \quad . \tag{16}$$

(ii) Reciprocal linear dispersion:

$$\left(\frac{\partial\lambda}{\partial(\Delta y')}\right)_{\alpha} = \frac{d\cos\beta}{mr'} \equiv \frac{10^{-3}\,d[\text{Å}]\cos\beta}{mr'[\text{m}]}\ \text{Å/mm} \quad . \tag{17}$$

(iii) Magnification:

$$M(\lambda) = \frac{\cos\alpha}{\cos\beta}\,\frac{r'}{r} \quad . \tag{18}$$

(iv) Phase-space acceptance (e):

$$\varepsilon = N\Delta\lambda_{S1} = N\Delta\lambda_{S2} \quad (\text{assuming } S_2 = MS_1) \quad , \tag{19}$$

where N is the number of participating grooves.

D. RESOLUTION PROPERTIES

The following are the main contributions to the width of the instrumental line spread function. An estimate of the total width is the vector sum.

(i) Entrance slit (width S_1):

$$\Delta\lambda_{S1} = \frac{S_1 d\cos\alpha}{mr} \quad . \tag{20}$$

(ii) Exit slit (width S_2):

$$\Delta\lambda_{S2} = \frac{S_2 d\cos\beta}{mr'} \quad . \tag{21}$$

(iii) Aberrations (of perfectly made grating):

$$\Delta\lambda_{\mathrm{A}} = \frac{\Delta y' d\cos\beta}{mr'} = \frac{d}{m}\left(\frac{\partial F}{\partial w}\right) \quad . \tag{22}$$

(iv) Slope error Δf (of imperfectly made grating):

$$\Delta\lambda_{SE} = \frac{d(\cos\alpha + \cos\beta)\Delta\phi}{m} \quad . \tag{23}$$

Note that, provided the grating is large enough, diffraction at the entrance slit always guarantees a coherent illumination of enough grooves to achieve the slit-width-limited resolution. In such case a diffraction contribution to the width need not be added to the above.

E. EFFICIENCY

The most accurate way to calculate grating efficiencies is by the full electromagnetic theory [8]. However, approximate scalar-theory calculations are often useful and, in particular, provide a way to choose the groove depth h of a laminar grating. According to Bennett, the best value of the groove-width-to-period ratio r is the one for which the usefully illuminated area of the groove bottom is equal to that of the top. The scalar-theory efficiency of a laminar grating with $r = 0.5$ is given by Franks et al. as

$$E_0 = \frac{R}{4}\left[1 + 2(1 - P)\cos\left(\frac{4\pi h\cos\alpha}{\lambda}\right) + (1 - P)^2\right]$$

$$E_m = \begin{cases} \dfrac{R}{m^2\pi^2}[1 - 2\cos Q^+ \cos(Q^- + \delta) \\ \quad + \cos^2 Q^+] & m = \text{odd} \\ \dfrac{R}{m^2\pi^2}\cos^2 Q^+ & m = \text{even} \end{cases} \tag{24}$$

where

$$P = \frac{4h\tan\alpha}{d_0} \quad ,$$

$$Q^{\pm} = \frac{m\pi h}{d_0}(\tan\alpha \pm \tan\beta) \quad ,$$

$$\delta = \frac{2\pi h}{\lambda}(\cos\alpha + \cos\beta) \quad ,$$

and R is the reflectance at grazing angle $\sqrt{\alpha_G\beta_G}$, where

$$\alpha_G = \frac{\pi}{2} - |\alpha| \text{ and } \beta_G = \frac{\pi}{2} - |\beta| \quad .$$

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