# X-Ray Data Booklet

## 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 $\alpha$ and $\beta$ have opposite signs if they are on opposite sides of the normal.

#### A.2 Grating equation

The grating equation may be written

$$m\lambda = d_0(\sin\alpha + \sin\beta). \quad (1)$$

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

(I) *ON-BLAZE CONDITION:*

$$\alpha + \beta = 2\theta_B, \quad (2)$$

where $\theta_B$ is the blaze angle (the angle of the sawtooth). The grating equation is then

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

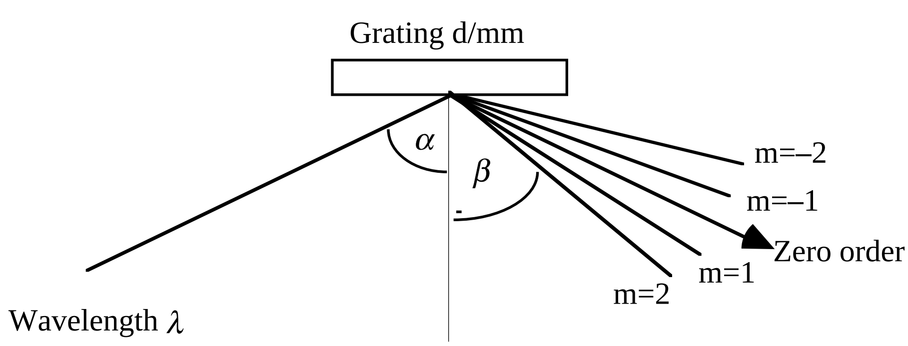


***Fig. 4-6.*** *Grating equation notation.*

(II) *FIXED IN AND OUT DIRECTIONS:*

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

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

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

In this case, the wavelength scan ends when $\alpha$ or $\beta$ reaches 90°, which occurs at the horizon wavelength $\lambda_H = 2d_0 \cos^2\theta$

(III) *CONSTANT INCIDENCE ANGLE*: EQUATION (1) GIVES $\beta$ DIRECTLY.

(IV) *CONSTANT FOCAL DISTANCE (OF A PLANE GRATING):*

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

leading to a grating equation

$$1 - \left(\frac{m\lambda}{d_0} - \sin\beta\right)^2 = \frac{\cos^2\beta}{c_{ff}^2} \tag{7}$$

Equations (3), (5), and (7) give $\beta$ (and thence $\alpha$) for any $\lambda$. Examples of the above $\alpha$-$\beta$ relationships are as follows:

(i) Kunz et al. plane-grating monochromator (PGM) [1], Hunter et al. double PGM[2], collimated-light SX700 [3]

(ii) Toroidal-grating monochromators (TGMs) [4, 5], spherical-grating monochromators (SGMs, “Dragon” system) [6], Seya-Namioka [7, 8] most aberration-reduced holographic SGMs [9], variable-angle SGM[10], PGMs [11, 12, 13]

(iii) Spectrographs, “Grasshopper” monochromator [14]

(iv) SX700 PGM [15] and variants [10, 16, 3]

## B. FOCUSING PROPERTIES [17]

The study of diffraction gratings[18, 19] goes back more than a century and has included plane, spherical [20, 21, 22], toroidal [23] and ellipsoidal[24] surfaces and groove patterns made by classical (“Rowland”) ruling [25], holography [26, 27, 28] and variably-spaced ruling [29]. In recent years the optical design possibilities of holographic groove patterns [30, 31, 32] and variably-spaced rulings [13] have been extensively developed. Following normal practice, we provide an analysis of the imaging properties of gratings by means of the path function $F$ [32]. 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 $n$th groove passes through the variable point P($w$,$l$). The holographic groove pattern is supposed to be made using two coherent point sources C and D with cylindrical polar coordinates $(r_C, \gamma, z_C)$, $(r_D, \delta, z_D)$ relative to O. The lower (upper) sign in eq. (9) refers

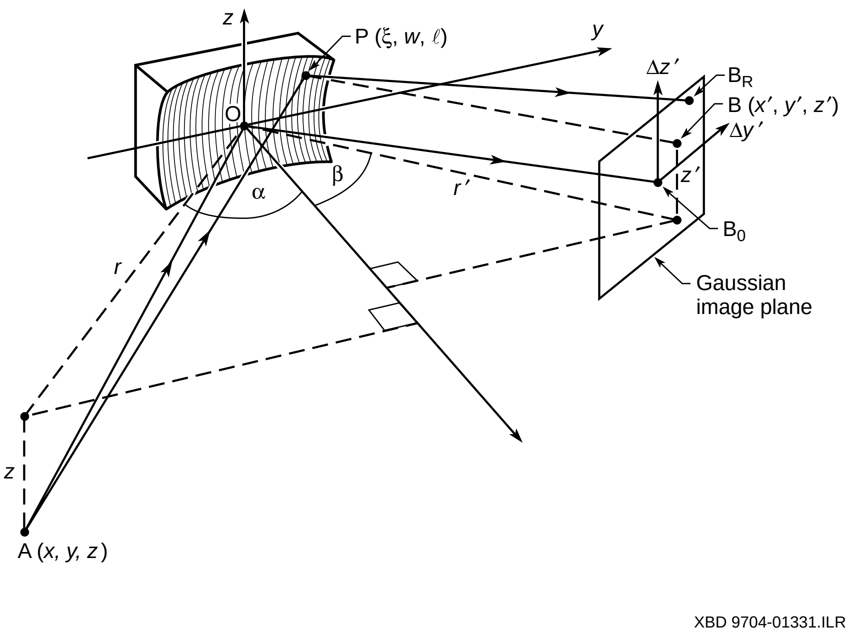


***Fig. 4-7*.*** *Focusing properties notation.*

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. The grating with varied line spacing $d(w)$ is assumed to be ruled according to $d(w) = d_0(1 + v_1 w + v_2 w^2 + \ldots)$. We consider all the gratings to be ruled on the general surface $x = \sum_{ij} a_{ij} w\, l$ and the $a_{ij}$ coefficients[33] are given for the important cases in Tables 1 and 2.

## B.1 Calculation of the path function *F*

$F$ is expressed as

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

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

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

$$f_{ijk} = \begin{cases} \delta_{(i-1)jk} & \text{Rowland} \\ \dfrac{d_0}{\lambda_0}\left\{ z_C^k C_{ijk}(\gamma, r_C) \pm z_D^k C_{ijk}(\delta, r_D) \right\} & \text{holographic} \\ n_{ijk} & \text{varied line spacing} \end{cases} \tag{9}$$

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 up to sixth order in Tables 3 and 4 in which the following notation is used:

$$T = T(r, \alpha) = \frac{\cos^2\alpha}{r} - 2a_{20}\cos\alpha \qquad S = S(r, \alpha) = \frac{1}{r} - 2a_{02}\cos\alpha \tag{10}$$

***Table 1:*** *Ellipse coefficients $Q_{ij}$ from which the $a_{ij}$'s are obtained*[a] *[33]*

| $j$ / $i$ | **0** | **1** | **2** | **3** | **4** | **5** | **6** |
|---|---|---|---|---|---|---|---|
| **0** | 0 | 0 | 1 | 0 | $C/4$ | 0 | $C^2/8$ |
| **1** | 0 | 0 | $A$ | 0 | $3AC/4$ | 0 | * |
| **2** | 1 | 0 | $(2A^2+C)/2$ | 0 | $3C(4A^2+C)/8$ | 0 | * |
| **3** | $A$ | 0 | $A(2A^2+3C)/2$ | 0 | * | 0 | * |
| **4** | $(4A^2+C)/4$ | 0 | $(8A^4+24A^2C+3C^2)/8$ | 0 | * | 0 | * |
| **5** | $A(4A^2+3C)/4$ | 0 | * | 0 | * | 0 | * |
| **6** | $(8A^4+12A^2C+C^2)/8$ | 0 | * | 0 | * | 0 | * |

[a]If $r,\ r'$ and $\theta$ are the object distance, image distance, and incidence angle to the normal, respectively, then

$$a_{ij} = a_{20}\frac{Q_{ij}}{\cos^j\theta} \quad \text{where} \quad a_{20} = \frac{\cos\theta}{4}\left(\frac{1}{r}+\frac{1}{r'}\right), \quad A = \frac{\sin\theta}{2}\left(\frac{1}{r}-\frac{1}{r'}\right), \quad C = A^2 + \frac{1}{rr'}$$

The $a_{ij}$'s for spheres, circular cylinders, paraboloids and hyperboloids can also be obtained from Tables 1 and 2 by suitable choices of the input parameters $r,\ r'$ and $\theta$.

***Table 2:*** *Toroid*[a] *$a_{ij}$'s [33]*

| $j$ / $i$ | **0** | **1** | **2** | **3** | **4** | **5** | **6** |
|---|---|---|---|---|---|---|---|
| **0** | 0 | 0 | $1/(2\rho)$ | 0 | $1/(8R^3)$ | 0 | $1/(16\rho^5)$ |
| **1** | 0 | 0 | 0 | 0 | 0 | 0 | * |
| **2** | $1/(2R)$ | 0 | $1/(4\rho R^2)$ | 0 | $(2\rho+R)/(16\rho^3R^3)$ | 0 | * |
| **3** | 0 | 0 | 0 | 0 | * | 0 | * |
| **4** | $1/(8R^3)$ | 0 | $3/(16\rho R^4)$ | 0 | * | 0 | * |
| **5** | 0 | 0 | * | 0 | * | 0 | * |
| **6** | $1/(16R^5)$ | 0 | * | 0 | * | 0 | * |

[a]$R$ and $\rho$ are the major and minor radii of the bicycle-tire toroid we are considering.

***Table 3:*** *Coefficients $C_{ijk}$ of the expansion of F* [a]

$$C_{011} = -\frac{1}{r} \qquad C_{020} = \frac{S}{2}$$

$$C_{022} = -\frac{S}{4r^2} - \frac{1}{2r^3} \qquad C_{031} = \frac{S}{2r^2}$$

$$C_{040} = \frac{4a_{02}^2 - S^2}{8r} - a_{04}\cos\alpha \qquad C_{042} = \frac{a_{04}\cos\alpha}{2r^2} + \frac{3S^2 - 4a_{02}^2}{16r^3} + \frac{3S}{4r^4}$$

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

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

$$C_{131} = -\frac{a_{12}\cos\alpha}{r^2} + \frac{3S\sin\alpha}{2r^3} \qquad C_{122} = \frac{a_{12}\cos\alpha}{2r^2} - \frac{3S\sin\alpha}{4r^3} - \frac{3\sin\alpha}{2r^4}$$

$$C_{200} = \frac{T}{2} \qquad C_{140} = -a_{14}\cos\alpha + \frac{1}{2r}\left(2a_{02}a_{12} + a_{12}S\cos\alpha - a_{04}\sin 2\alpha\right) + \frac{\sin\alpha}{8r^2}\left(4a_{02}^2 - 3S^2\right)$$

$$C_{202} = -\frac{T}{4r^2} + \frac{\sin^2\alpha}{2r^3} \qquad C_{211} = \frac{T}{2r^2} - \frac{\sin^2\alpha}{r^3}$$

$$C_{013} = \frac{1}{2r^3} \qquad C_{300} = -a_{30}\cos\alpha + \frac{T\sin\alpha}{2r}$$

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

$$C_{222} = \frac{1}{2r^2}a_{22}\cos\alpha + \frac{1}{8r^3}\left(3ST - 4a_{02}a_{20} + 6a_{12}\sin 2\alpha\right) + \frac{3}{4r^4}\left(T - 2S\sin^2\alpha\right) - \frac{3\sin^2\alpha}{r^5}$$

$$C_{231} = -\frac{1}{r^2}a_{22}\cos\alpha + \frac{1}{4r^3}\left(-3ST + 4a_{02}a_{20} - 6a_{12}\sin 2\alpha\right) + \frac{3S\sin^2\alpha}{r^4}$$

$$C_{240} = -a_{24}\cos\alpha + \frac{1}{2r}\left(a_{12}^2\sin^2\alpha + 2a_{04}a_{20} + a_{22}S\cos\alpha + a_{04}T\cos\alpha - a_{14}\sin 2\alpha + 2a_{02}a_{22}\right)$$
$$+ \frac{1}{16r^2}\left(-4a_{02}^2T - 8a_{02}a_{20}S + 12a_{12}S\sin 2\alpha + 3TS^2 + 16a_{02}a_{12}\sin\alpha - 8a_{04}\sin 2\alpha\right) + \frac{\sin^2\alpha}{4r^3}\left(2a_{02}^2 - 3S^2\right)$$

$$C_{302} = \frac{a_{30}\cos\alpha}{2r^2} - \frac{3T\sin\alpha}{4r^3} + \frac{\sin^3\alpha}{2r^4}$$

$$C_{311} = -\frac{a_{30}\cos\alpha}{r^2} + \frac{3T\sin\alpha}{2r^3} - \frac{\sin^3\alpha}{r^4}$$

***Table 3:** Coefficients $C_{ijk}$ of the expansion of $F$ [a] (continued)*

$$C_{320} = -a_{32}\cos\alpha + \frac{1}{2r}\left(2a_{20}a_{12} + 2a_{30}a_{02} + a_{30}S\cos\alpha + a_{12}T\cos\alpha - a_{22}\sin 2\alpha\right)$$
$$+ \frac{1}{4r^2}\left(4a_{20}a_{02}\sin\alpha - 3ST\sin\alpha - 4a_{12}\cos\alpha\sin^2\alpha\right) + \frac{S\sin^3\alpha}{2r^3}$$

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

$$C_{402} = -\frac{1}{16r^3}\left(4a_{20}^2 + 3T^2 + 12a_{30}\sin 2\alpha\right) + \frac{a_{40}\cos\alpha}{2r^2} - \frac{3T\sin^2\alpha}{2r^4} + \frac{\sin^4\alpha}{2r^5}$$

$$C_{411} = -\frac{a_{40}\cos\alpha}{r^2} + \frac{1}{8r^3}\left(4a_{20}^2 - 3T^2 - 12a_{30}\sin 2\alpha\right) + \frac{3T\sin^2\alpha}{r^4} - \frac{\sin^4\alpha}{r^5}$$

$$C_{420} = -a_{42}\cos\alpha + \frac{1}{2r}\left(2a_{20}a_{22} + 2a_{12}a_{30}\sin^2\alpha + 2a_{02}a_{40} - a_{32}\sin 2\alpha + a_{40}S\cos\alpha + a_{22}T\cos\alpha\right)$$
$$+ \frac{1}{16r^2}\left(-4a_{20}^2S - 8a_{02}a_{20}T + 3ST^2 + 12\sin 2\alpha\left(a_{30}S + a_{12}T\right) + 8\sin\alpha\left(2a_{02}a_{30} - 2a_{22}\sin 2\alpha + 2a_{12}a_{20}\right)\right)$$
$$+ \frac{1}{2r^3}\left(2a_{02}a_{20}\sin^2\alpha - 3ST\sin^2\alpha - 2a_{12}\cos\alpha\sin^3\alpha\right) + \frac{S\sin^4\alpha}{2r^4}$$

$$C_{500} = -a_{50}\cos\alpha + \frac{1}{2r}\left(2a_{20}a_{30} + a_{30}T\cos\alpha - a_{40}\sin 2\alpha\right) + \frac{\sin\alpha}{2r^2}\left(a_{20}^2 - a_{30}\sin 2\alpha\right) - \frac{3T^2\sin\alpha}{8r^2} + \frac{T\sin^3\alpha}{2r^3}$$

$$C_{600} = -a_{60}\cos\alpha + \frac{1}{2r}\left(a_{30}^2\sin^2\alpha + 2a_{20}a_{40} + a_{40}T\cos\alpha - a_{50}\sin 2\alpha\right)$$
$$+ \frac{1}{16r^2}\left(-4a_{20}^2T + T^3 + 16a_{20}a_{30}\sin\alpha + 12a_{30}T\sin 2\alpha - 16a_{40}\cos\alpha\sin^2\alpha\right)$$
$$+ \frac{1}{4r^3}\left(2a_{20}^2\sin^2\alpha - 3T^2\sin^2\alpha - 4a_{30}\cos\alpha\sin^3\alpha\right) + \frac{T\sin^4\alpha}{2r^4}$$

[a]The coefficients for which $i \le 6, j \le 4, k \le 2, i + j + k \le 6, j + k = \text{even}$ are included in this table. The only addition to those is $C_{013}$, which has some interest, because, when the system is specialized to be symmetrical about the *x* axis, it represents a Seidel aberration, namely distortion.

***Table 4:*** *Coefficients $n_{ijk}$ of the expansion of F for a grating with variable line spacing*

| | |
|---|---|
| $n_{ijk}=0 \quad \text{for} \quad j,k \neq 0$ | |
| $n_{100}=1$ | $n_{400}=\left(-v_1^3+2v_1v_2-v_3\right)\big/4$ |
| $n_{200}=-v_1/2$ | $n_{500}=\left(v_1^4-3v_1^2v_2+v_2^2+2v_1v_3-v_4\right)\big/5$ |
| $n_{300}=\left(v_1^2-v_2\right)\big/3$ | $n_{600}=\left(-v_1^5+4v_1^3v_2-3v_1v_2^2-3v_1^2v_3+2v_2v_3+2v_1v_4-v_5\right)\big/6$ |

### B.2 Determination of the Gaussian image point

By definition the principal ray $AOB_0$ arrives at the Gaussian image point $B_0(r_0',\beta_0,z_0')$ (Fig. 4.7) and its direction is given by Fermat's principal which implies $\lfloor \partial F/\partial w \rfloor_{w=0,l=0}=0, \quad \lfloor \partial F/\partial l \rfloor_{w=0,l=0}=0$ whence

$$\frac{m\lambda}{d_0}=\sin\alpha+\sin\beta_0, \quad \frac{z}{r}+\frac{z_0'}{r_0'}=0 \quad , \tag{11}$$

The tangential focal distance $r_0'$ is obtained by setting the focusing term $F_{200}$ equal to zero and is given by

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

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

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

which has important special cases. (i) plane grating, $R=\infty$ implying $r_0'=-r\cos^2\alpha\big/\cos^2\beta$, (ii) object and image on the Rowland circle, or $r=R\cos\alpha$, $r_0'=R\cos\beta$ and $M=1$ and (iii) $\beta$=90° (Wadsworth condition). The focal distances of TGMs and SGMs are also determined by 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 [34, 35, 36]

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

where $F$ is to be evaluated for $A = (r, \alpha, z)$, $B = (r_0', \beta_0, z_0')$. By means of the expansion of $F$, these equations allow the ray aberrations to be calculated separately for each aberration type.

$$\Delta y'_{ijk} = \frac{r_0'}{\cos\beta_0}F_{ijk}iw^{i-1}l^j, \qquad \Delta z'_{ijk} = r_0'F_{ijk}w^i jl^{j-1}. \tag{15}$$

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

## C. DISPERSION PROPERTIES

### C.1 Angular dispersion

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

### C.2 Reciprocal linear dispersion

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

### C.3 Magnification (*M*)

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

### C.4 Phase-space acceptance ($\varepsilon$)

$$\varepsilon = N\Delta\lambda_{S_1} = N\Delta\lambda_{S_2} \quad (\text{assuming } S_2 = MS_1) \tag{19}$$

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. The actual width is the vector sum.

(I) *ENTRANCE SLIT (WIDTH $S_1$):*

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

(II) *EXIT SLIT (WIDTH $S_2$):*

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

(III) *ABERRATIONS (OF PERFECTLY MADE GRATING):*

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

(IV) *SLOPE ERROR $\Delta\phi$* (*OF IMPERFECTLY MADE GRATING*):

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

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 and a diffraction contribution to the width need not be added to the above.

## 1. EFFICIENCY

The most accurate way to calculate grating efficiencies is by the full electromagnetic theory [37, 38] for which a code is available from Neviere. 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 [39], the best value of the groove-width-to-period ratio (*r*) is the one for which the usefully illuminated groove area is equal to the land area. The scalar theory efficiency of a laminar grating with *r*=0.5 is given by [40]

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

$$E_m = \begin{cases} \dfrac{R}{m^2\pi^2}\left\{1 - 2\cos Q^+ \cos\left(Q^- + \delta\right) + \cos^2 Q^+\right\} & m = \text{odd} \\ \dfrac{R}{m^2\pi^2}\cos^2 Q^+ & m = \text{even} \end{cases}$$

where

$$P = \frac{4h\tan\alpha}{d_0}, \quad Q^\pm = \frac{m\pi h}{d_0}(\tan\alpha \pm \tan\beta), \quad \delta = \frac{2\pi h}{\lambda}(\cos\alpha + \cos\beta) \tag{24}$$

and $R$ is the reflectance at angle $\sqrt{\alpha\beta}$.

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