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FINAL REPORT

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THE NATIONAL AERONATICS AND SPACE AGENCY

FOR

HOLOGRAPHIC GRATINGS FOR SPECTOROGRAPHIC APPLICATIONS:

STUDY OF ABBERATIONS

(CONTRACT NO. NGR-21-027-010)

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This is the final report of the project entitled "Holographic Gratings for Spectrographic Applications: Study of Abberations" conducted at Bowie State College with the help of faculty and students.

This report is divided into the following independent parts, each of which can be studied separately:

1. Computer Program for Designing Holographic Gratings for Seya-Namioka Type Monochromators: Part I: Minimization of Abberations Over a Desired Wavelength Range.

2. Computer Program for Designing Holographic Gratings for Seya-Namioka Type Monochromators: Part I: Correcting Abberations at Specified Wavelengths.

3. Design of Astigmatism or Coma Corrected Holographic Gratings for Rowland Circle Spectrographic Mounts.

4. Simultaneous Correction of Astigmatism. Coma. and First Spherical Abberation Term of Holographic Concave Gratings for Rowland Circle Spectrographs.

5. Design of Abberation Corrected Holographic Toroid Gratings for Seya-Namioka Type Monochromators.

This report concludes this project.

COMPUTER PROGRAM FOR DESIGNING HOLOGRAPHIC GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

PART I: MINIMIZATION OF ABERRATIONS OVER A DESIRED WAVELENGTH RANGE

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COMPUTER PROGRAM FOR DESIGNING HOLOGRAPHIC GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

INTRODUCTION

A computer program has been developed based on the theory presented in papers by Greiner and Schaeffer (Reference 1) and Noda-Namioka and Seya (Reference 2), that determines the optimum holographic grating recording parameters as a function of optical instrumental parameters and desired wavelength range for Seya-Namioka monochromator mountings. The report is divided into two parts. In Part I, the holographic grating recording parameters are determined such that astigmatism or coma may be minimized over a selected wavelength range, and in Part II, we determine optimum recording parameters such that astigmatism or coma may be corrected to zero at specified wavelengths within the desired wavelength range. The program also simultaneously displays the performance of the holographic grating and equivalent conventional grating as a function of wavelength relative to optical aberrations of astigmatism, coma, and spherical aberration.

In this report two methods of designing holographic gratings for operation in negative orders only have been developed. The first method is the GENERAL METHOD, and with this method the instrumental constants are related only to the holographic grating. The second method is called the MODIFIED METHOD, and with this method it is possible to design holographic gratings that minimize astigmatism or coma over a desired wavelength range for Seya-Namioka monochromators that are interchangeable with conventional gratings. This means that the instrumental constants are the same for both holographic gratings and conventional gratings.

The contents of this report are divided into four sections. Section I presents the theory and basic equations for designing holographic concave gratings such that minimization of aberrations of astigmatism or coma over a desired wavelength range may be achieved. The basic equations are extracted from Reference 2 and are presented so that a better understanding of the computer program may be appreciated. For more detailed theoretical analysis see Reference 2. A description of the computer program including all of the subroutines is presented in Section 2. Section 3 presents the input data, definition of terms and data card description. Section 4 presents an example for using the program and describes the output data in detail.

SECTION 1. THEORY AND BASIC EQUATIONS FOR DESIGNING HOLOGRAPHIC CONCAVE GRATINGS

Since a detailed theoretical explanation relative to the design of holographic concave gratings is given in Reference 2, we only present a brief description for ease of understanding the development of the computer program presented in this report.

Figure 1 shows a schematic diagram of the optical system which defines a rectangular coordinate system. We have used the same terminology as Noda, Namioka, and Seya (Reference 2) in order to avoid any ambiguity. Let the origin be at vertex O of the concave grating having a radius of curvature R. Let the x-axis be the normal to the grating at O and let the xy plane be defined by O and two coherent point sources C and D used to record the interference fringes on a concave substrate. Points A, P, and B are self-luminous points on the entrance slit; a point on the grating and a point at the focus of the diffracted image from P of wavelength λ in the m-th order, respectively.

For the ray APB, the light path function F is given by

$$\begin{aligned} F = {} & F_{000} + wF_{100} + LF_{011} + \tfrac{1}{2} w^2 F_{200} \\ & + \tfrac{1}{2} L^2 F_{020} + \tfrac{1}{2} w^3 F_{300} + \tfrac{1}{2} wL^2 F_{120} + wLF_{111} \\ & + \tfrac{1}{8} w^4 F_{400} + \tfrac{1}{4} w^2 L^2 F_{220} + \tfrac{1}{8} L^4 F_{040} + \tfrac{1}{4} wL^2 F_{202} \\ & + \tfrac{1}{4} L^2 F_{022} + \tfrac{1}{2} L^3 F_{031} + \tfrac{1}{2} w^2 LF_{211} + \cdots \end{aligned} \tag{1}$$

and

$$F_{ijk} = M_{ijk} + \left(\frac{m\lambda}{\lambda_0}\right) H_{ijk} \tag{2}$$

The M terms refer to the contribution of the conventionally ruled grating and the H terms refer to the contribution of the holographic grating. In equation (2), m is the order of the grating, λ_0 is the laser radiation wavelength, and λ is the wavelength at which the grating is being employed. The terms M_{ijk} and H_{ijk} are defined in terms of the functions f_{ijk} as follows:

$$\begin{aligned} M_{ijk} &= f_{ijk}(\rho,\alpha) + f_{ijk}(\rho',\beta), \\ H_{ijk} &= f_{ijk}(\rho_C,\gamma) - f_{ijk}(\rho_D,\delta) \end{aligned} \tag{3}$$

for (ijk) = (200), (020), (300), (120),

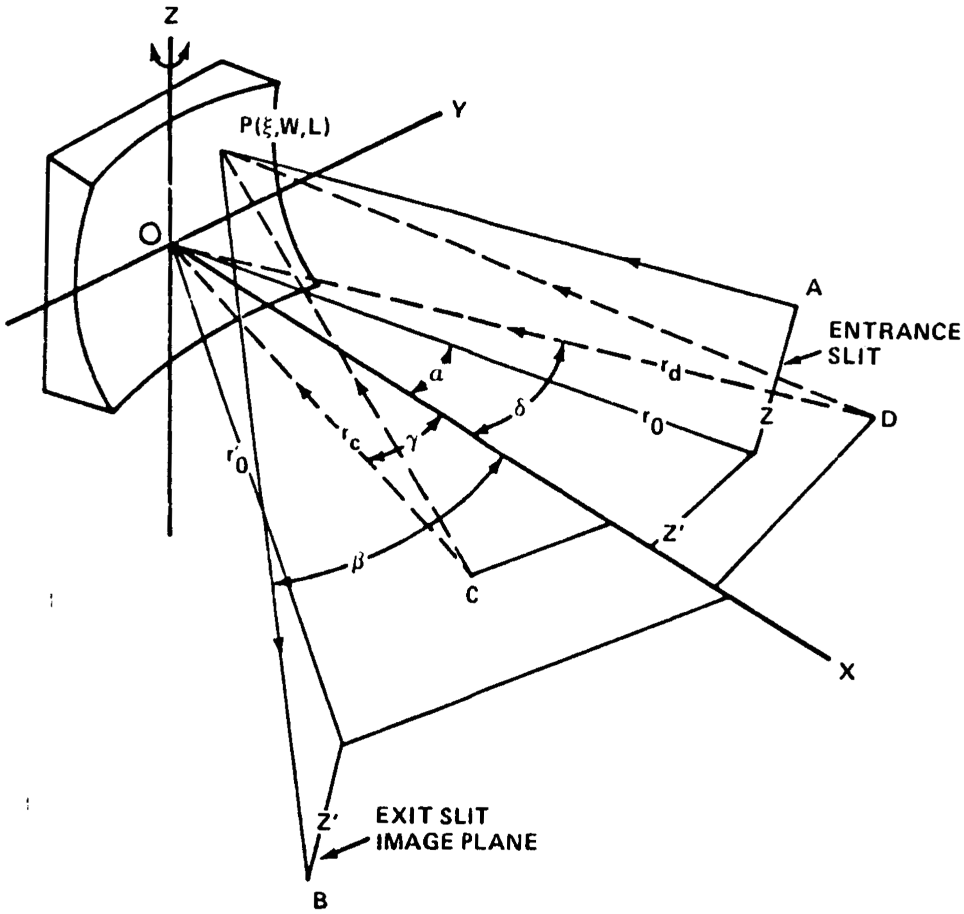

Figure 1. Schematic diagram showing the geometry for recording the holographic grating. The instrumental and recording parameters are defined as follows:

Instrument Parameters

- r_0 is the object distance from the entrance slit to the center of the grating.
- r'_0 is the image distance from the exit slit to the center of the grating.
- α is the angle of incident radiation relative to the normal of the grating.
- β is the diffracted image angle relative to the normal of the grating.
- A is the entrance slit position and B is the exit slit position.

Recording Parameters

- r_C is the distance of recording point source C to the center of the grating.
- r_D is the distance of the recording point source D to the center of the grating.
- δ is the recording angle for positioning point source D relative to the normal of the grating.
- γ is the recording angle for positioning point source C relative to the normal of the grating.

$$M_{ijk} = M_{020} - (-1)^{\frac{1}{2}i} [f_{ijk}(\rho,\alpha) + f_{ijk}(\rho',\beta)],$$
$$H_{ijk} = H_{020} - (-1)^{\frac{1}{2}i} [f_{ijk}(\rho_C,\gamma) - f_{ijk}(\rho_D,\delta)] \quad (4)$$

for (ijk) = (400), (220), (040), where

$$\begin{aligned}
f_{200}(\rho,\alpha) &= (\rho\cos\alpha - 1)\cos\alpha, \\
f_{020}(\rho,\alpha) &= \rho - \cos\alpha, \\
f_{300}(\rho,\alpha) &= \rho\sin\alpha \cdot f_{200}(\rho,\alpha), \\
f_{120}(\rho,\alpha) &= \rho\sin\alpha \cdot f_{020}(\rho,\alpha), \\
f_{400}(\rho,\alpha) &= \rho f_{200}(\rho,\alpha)\,[f_{200}(\rho,\alpha) - 4\rho\sin^2\alpha], \\
f_{220}(\rho,\alpha) &= \rho f_{020}(\rho,\alpha)\,[2\rho\sin^2\alpha - f_{200}(\rho,\alpha)], \\
f_{040}(\rho,\alpha) &= \rho\,[f_{020}(\rho,\alpha)]^2
\end{aligned} \quad (5)$$

$$\rho = R/r, \quad \rho' = R/r', \quad \rho_C = R/r_C, \quad \rho_D = R/r_D, \quad (6)$$

$$x = r\cos\alpha, \quad y = r\sin\alpha, \quad x' = r'\cos\beta, \quad y' = r'\sin\beta,$$

$$x_C = r_C\cos\gamma, \quad y_C = r_C\sin\gamma, \quad x_D = r_D\cos\delta, \quad y_D = r_D\sin\delta. \quad (7)$$

For equations (2)-(7), R is the radius of curvature of the grating and (r_C, γ, O) and (r_D, δ, O) are respectively the cylindrical coordinates of the point sources C and D.

The grating equation is given by

$$\sigma(\sin\alpha_0 + \sin\beta_0) = m\lambda \quad (8)$$

for the principal ray, the ray originating from the center of the entrance slit, and diffracted from O at an angle β. σ is the effective grating constant defined by

$$\sigma = \frac{\lambda_0}{\sin\delta - \sin\gamma}, \quad (9)$$

where $\delta > \gamma$. Note that the number of grooves per unit length is $N = 1/\sigma$.

Minimization of Aberration Terms

The theory described up to this point has been presented for the general case. We now apply the general theory to a specific application: the Seya-Namioka monochromator. For the Seya-Namioka monochromator the basic instrumental parameters are defined as follows (Reference 2); see Figure 2.

$$r_0, \bar{r}'_0 = \text{constant}, \quad 2\kappa = \alpha_0 - \beta_0 = \text{constant}$$
$$\alpha_0 = \kappa + \theta, \qquad \beta_0 = \theta - \kappa \tag{10}$$

where r_0 is the distance from the center of the entrance slit to O and $\bar{r}'_0$ is the distance from O to the center of the exit slit. 2κ is the angle AOB and θ is the angle of grating rotation measured from the bisector of the angle 2κ and has the same sign as the spectral order m. Under conditions (10), the relation between θ and λ is given by

$$\lambda = \left(\frac{2\sigma}{m}\right)\cos\kappa \sin\theta \tag{11}$$

We denote F_{ijk} for the ray AOB by $\bar{F}_{ijk}$. Then, the aberrations in the Seya-Namioka monochromator can be reduced by minimizing the functions

$$\begin{aligned} \bar{F}_{ijk}(\bar{\rho}, \bar{\rho}', \theta, \kappa, A_{ijk}) &= \bar{M}_{ijk} + \left(\frac{m\lambda}{\lambda_0}\right) H_{ijk} \\ &= \bar{M}_{ijk} + A_{ijk}(\sin\alpha_0 + \sin\beta_0) \end{aligned} \tag{12}$$

where $i + j + k \geqslant 2$ over a predetermined scanning range, $\theta_1 \leqslant \theta \leqslant \theta_2$ or $\lambda_1 \leqslant \lambda \leqslant \lambda_2$ where

$$\bar{\rho} = \frac{R}{r_0}, \quad \bar{\rho}' = \frac{R}{\bar{r}'} = \frac{R}{r'_0}, \tag{13}$$

$$A_{ijk} = \frac{H_{ijk}}{\sin\delta - \sin\gamma} = \left(\frac{\sigma}{\lambda_0}\right) H_{ijk} \tag{14}$$

and θ_1, and θ_2 are related to λ_1 and λ_2 through equation (11). This is equivalent to imposing on $\bar{F}_{ijk}$'s the condition

$$I_{ijk} \equiv \int_{\theta_1}^{\theta_2} \bar{F}^2_{ijk}\, d\theta = \text{minimum} \tag{15}$$

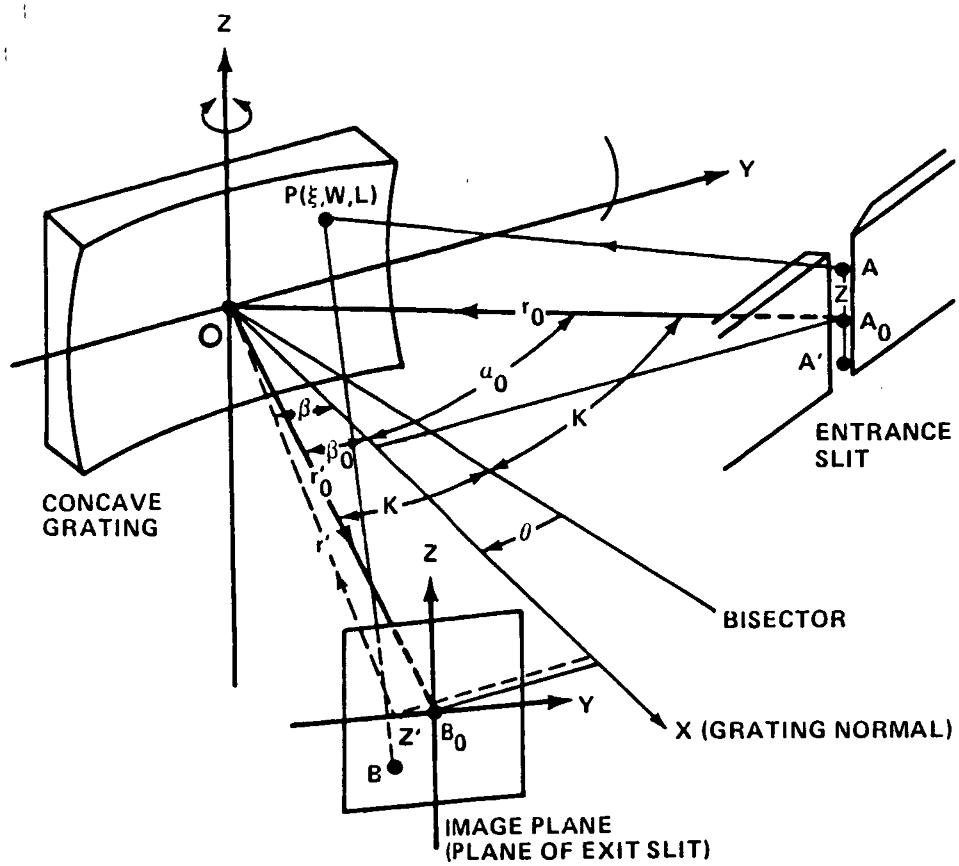

Figure 2. Schematic Diagram of the Optical System for Seya-Namioka Monochromator

Determination of Instrumental Parameters $\bar{\rho}$, $\bar{\rho}'$, κ and A_{200}

The optimum instrumental parameters are determined in such a way that equation (15) is satisfied for the horizontal focusing condition $\bar{F}_{200}$. This is accomplished by solving the following equations simultaneously,

$$\frac{\partial I_{200}}{\partial \bar{\rho}} = 0, \quad \frac{\partial I_{200}}{\partial \bar{\rho}'} = 0,$$

$$\frac{\partial I_{200}}{\partial \kappa} = 0, \quad \frac{\partial I_{200}}{\partial A_{200}} = 0. \tag{16}$$

Once the optimum values of $\bar{\rho}, \bar{\rho}'$ and κ are determined, then each one of the integrals I_{ijk} with $i + j + k \geqslant 2$ becomes a function only of A_{ijk}. Then, those values of A_{ijk}'s which satisfy equation (15) are calculated from the equation

$$\frac{\partial I_{ijk}}{\partial A_{ijk}} = 0$$

where

$$A_{ijk} = [B_{ijk}(\theta_2) - B_{ijk}(\theta_1)] \,/\, [2(\theta_2 - \theta_1) - (\sin 2\theta_2 - \sin 2\theta_1)] \cos\kappa \tag{17}$$

where

$$\begin{aligned} B_{200}(\theta) = {} & (\bar{\rho}/3)[\cos\theta + \cos(\theta+\kappa)\cos(2\theta+\kappa) \\ & + 3\sin(\theta+\kappa)\sin\kappa] \\ & + (\bar{\rho}'/3)[\cos\theta + \cos(\theta-\kappa)\cos(2\theta-\kappa) \\ & - 3\sin(\theta-\kappa)\sin\kappa] - \cos 2\theta\cos\kappa, \end{aligned} \tag{18}$$

$$B_{020}(\theta) = 2(\bar{\rho} + \bar{\rho}')\cos\theta - \cos 2\theta\cos\kappa, \tag{19}$$

$$\begin{aligned} B_{300}(\theta) = {} & (\bar{\rho}/4)^2[\sin(4\theta+3\kappa) - 4\cos 2(\theta+\kappa)\sin\kappa - 4\theta\cos\kappa] \\ & + (\bar{\rho}'/4)^2[\sin(4\theta-3\kappa) + 4\cos(\theta-\kappa)\sin\kappa - 4\theta\cos\kappa] \\ & + (\bar{\rho}/6)[3\sin(\theta+2\kappa) - \sin(3\theta+2\kappa)] \\ & + (\bar{\rho}'/6)[3\sin(\theta-2\kappa) - \sin(3\theta-2\kappa)], \end{aligned} \tag{20}$$

$$\begin{aligned} B_{120}(\theta) = {} & \tfrac{1}{2}\,\bar{\rho}^2[\sin(2\theta+\kappa) - 2\theta\cos\kappa] \\ & + \tfrac{1}{2}\,\bar{\rho}'^2[\sin(2\theta-\kappa) - 2\theta\cos\kappa] \\ & + (\bar{\rho}/6)[3\sin(\theta+2\kappa) - \sin(3\theta+2\kappa)] \\ & + (\bar{\rho}'/6)[3\sin(\theta-2\kappa) - \sin(3\theta-2\kappa)], \end{aligned} \tag{21}$$

and so on.

Determination of the Recording Parameters ρ_C, ρ_D, γ and δ and Minimization of Astigmatism or Coma

The recording parameters are dependent upon the aberrations to be minimized. With a predetermined effective grating constant, the following equations are solved simultaneously for minimizing astigmatism and one coma-type aberration,

$$\begin{aligned} \sin\delta - \sin\gamma &= \lambda_0/\sigma, \\ f_{200}(\rho_C,\gamma) - f_{200}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{200}, \\ f_{020}(\rho_C,\gamma) - f_{020}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{020}, \\ f_{300}(\rho_C,\gamma) - f_{300}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{300}; \end{aligned} \tag{22}$$

and for minimizing coma-type aberrations

$$\begin{aligned} \sin\delta - \sin\gamma &= \lambda_0/\sigma, \\ f_{200}(\rho_C,\gamma) - f_{200}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{200}, \\ f_{300}(\rho_C,\gamma) - f_{300}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{300}, \\ f_{120}(\rho_C,\lambda) - f_{120}(\rho_D,\delta) &= (\lambda_0/\sigma)A_{120}. \end{aligned} \tag{23}$$

Before making any attempt to solve equation (22) or (23) it is necessary to investigate the conditions under which equation (22) or (23) can have real solutions for ρ_C and ρ_D because H_{300} and H_{120} are quadratic in ρ_C and ρ_D and their values depend on A_{300} and A_{120} and therefore on values of θ_2 in I_{300} and I_{120}. The condition may be stated in such a way that two quadratic equations of ρ_C or ρ_D resulting from equations (22) and (23) should not have imaginary roots. To fulfill this condition, A_{300} and A_{120} must satisfy the equation

$$b^2 - 4ac \geqslant 0 \tag{24}$$

where for A_{300}

$$\begin{aligned} a &= (\sin\delta\cos^2\gamma - \sin\gamma\cos^2\delta)\cos^2\gamma, \\ b &= [2\rho\cos\gamma\sin\delta + \sin(\delta-\gamma)\cos\delta]\cos\gamma, \\ c &= \rho(\rho+\cos\delta)\sin\delta + A_{300}\cos^2\delta(\sin\delta - \sin\gamma), \end{aligned} \tag{25}$$

and for A_{120}

$$
\begin{aligned}
a &= \cos^4 \gamma \sin \delta - \sin \gamma \cos^4 \delta, \\
b &= [2\rho \cos \gamma \sin \delta + \sin (\delta - \gamma) \cos^3 \delta] \cos \gamma, \\
c &= \rho (\rho \sin \delta + \cos^3 \delta) \sin \delta + A_{120} \cos^4 \delta (\sin \delta - \sin \gamma);
\end{aligned} \tag{26}
$$

$$
\rho = A_{200}(\sin \delta - \sin \gamma) + \cos \gamma - \cos \delta. \tag{27}
$$

When condition (24) is satisfied, then ρ_C and ρ_D are solutions to equations (22) and (23)

Up to this point, we have been describing the general method of designing aberration corrected holographic gratins for Seya-Namioka monochromators which are not interchangeable with conventional gratings.

Modified Method

The modified method of designing holographic gratings for the Seya-Namioka monochromator has a practical advantage in that the holographic grating is interchangeable with a conventionally ruled grating having the same radius of curvature. This is possible provided the same instrumental constants $\bar{\rho}$, $\bar{\rho}'$ and κ used for the conventionally ruled grating are used to design the holographic grating. The instrumental constants for the conventional grating are determined by solving the equation

$$
I_{200} \equiv \int_{\theta_1}^{\theta_2} \bar{M}_{200}^2 \, d\theta = \text{minimum}
$$

or

$$
\frac{\partial I_{200}}{\partial \bar{\rho}} = 0, \quad \frac{\partial I_{200}}{\partial \bar{\rho}'} = 0
$$

and

$$
\frac{\partial I_{200}}{\partial \kappa} = 0 \tag{28}
$$

The design procedure given by equations (15)-(23) must be modified in part in order to accommodate condition (28). The modification required is to replace equation (16) with equation (28) and equation (17) with (ijk) = (200) and the rest of the procedure remains the same.

SECTION 2

Section 1 described the theory of designing holographic gratings that minimize aberrations over a selected wavelength range. In this section, we use the theory and present the computer program which consists of a main program and four subroutines. Figure 3 is a diagram of the flow chart for the program.

PROGRAM DESCRIPTION

The following is a presentation of the main program and algorithms for each subroutine in the computer program to show how the algorithms perform their specific tasks.

MAIN PROGRAM

The purpose of this program is to direct the flow of calculations depending upon which option is selected. If option LMN = 2 is selected, then the optimum value of the instrumental parameter angle 2κ will be calculated. However, if the program user chooses to specify an angle 2κ as an input value then option LMN = 1 is used.

The computer program has been developed to accommodate two holographic grating design methods; the general method and the modified method. If the general method is selected, then the option called IETA = 1 is used in the program. When using option IETA = 1, all the instrumental parameters are related only to the holographic grating.

If the modified method is selected, then option IETA = 0 is used in the program. When using this option, all instrumental parameters calculated are the same for both holographic and conventional gratings. This means that the holographic and conventional gratings are interchangeable if they have the same groove frequency and radius of curvature. The only difference is that the holographic grating minimizes aberrations and the conventional grating does not.

Once the design method has been selected and the LMN option has been chosen, the following steps of calculation are performed.

STEP A: Read input cards.

STEP B: Call INSTRM to calculate the optimum angle 2κ, and then calculate B_{ijk} and A_{ijk} (equation (17) (LMN = 2)) or calculate the functions B_{ijk} and A_{ijk} using the input value of 2κ (LMN = 1).

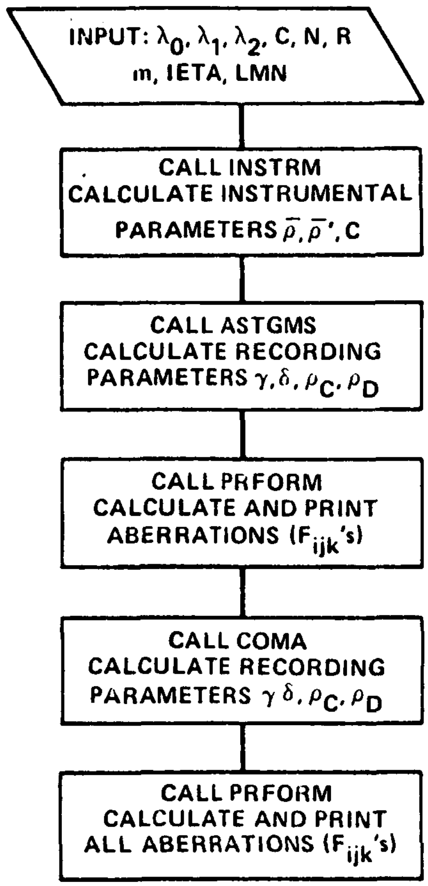

Figure 3. Main Program Flow Chart

STEP C: Call ASTGMS to calculate the recording parameters ρ_C, ρ_D, γ, and δ to minimize astigmatism ijk = (020) and one coma term ijk = (300).

STEP D: Call COMA to calculate the recording parameters ρ_C, ρ_D, γ, and δ to minimize coma aberrations (ijk) = (300) and (ijk) = (120).

STEP E: Call PRFORM to display the numerical values of each aberration of the holographic grating and compare with that of the equivalent conventional grating as a function of wavelength. Note that the program automatically calculates the recording parameters for both the astigmatism minimization and coma minimization. This feature was included in the program so that the program user may select which aberration minimization will best produce the optimum minimization for all aberrations (astigmatism, coma and spherical) throughout the desired wavelength range.

Subroutine INSTRM

This subroutine obtains the optimum values of the instrumental parameters, namely $\bar{\rho}$, $\bar{\rho}'$, 2κ and A_{200} by simultaneous solution of equation (16). A modified form of Newton's method is used to obtain the solution. The quantities B_{ijk} are then calculated using the optimum values of $\bar{\rho}$, $\bar{\rho}'$, and 2κ which in turn give A_{ijk} by equation (17). If a prescribed input value of 2κ were used, the selection of option LMN = 1 would by-pass the optimization procedures when calculating the other instrumental parameters.

The values of the instrumental parameters as well as A_{300}, A_{020}, and A_{120} are printed at the end of this subroutine.

Subroutine ASTGMS

The purpose of this subroutine is to obtain the recording parameters such that astigmatism (ijk) = (020) and a coma type term (ijk) = (300) are minimized over the given wavelength range $\lambda_1 \leqslant \lambda \leqslant \lambda_2$. This is achieved by finding a simultaneous solution of equation (22).

It is first verified that the quantity $N\lambda_0$ is less than the maximum value of $|(\sin \delta - \sin \gamma)|$, namely 2. If not, an error message is printed stating "error, GAMA out of bounds."

The values of a, b, c of equation (25) or (26) are then computed and the discriminant is checked to ensure $b^2 - 4ac \geqslant 0$. The solutions of the quadratic equation aré computed and are checked for positiveness; the calculations show that one of the two roots $[(-b \pm \sqrt{b^2 - 4ac})/2a]$ is always positive and the other always negative.

The value of the angle γ to the desired accuracy is determined by the iterated solution of the equation (22) by Newton's method. The resulting values of the recording parameters γ and δ are printed at the end of this subroutine.

Subroutine COMA

The purpose of this subroutine is to obtain the recording parameters such that the coma type terms (ijk) = (300) and (120) are minimized over a given wavelength range $\lambda_1 \leqslant \lambda \leqslant \lambda_2$. This is achieved by finding a simultaneous solution of equation (23).

It is first verified that the quantity $N\lambda_0$ is less than the maximum value of $|(\sin \delta - \sin \gamma)|$, namely 2. If not, an error message is printed stating "error, GAMA out of bounds."

The values of a, b, c of equation (25) or (26) are then computed and the discriminant is checked to ensure that $b^2 - 4ac \geqslant 0$. The solutions of the quadratic equation are computed and are verified for positiveness; the calculations show that one of the two roots $[(-b + \sqrt{b^2 - 4ac})/2a]$ is always positive and the other always negative.

The value of the angle γ to the desired accuracy is determined by the iterated solution of the equation (22) by Newton's method. The resulting values of the recording parameters γ and δ are printed at the end of this subroutine.

Subroutine PRFROM

This subroutine calculates the performance of the holographic grating with the recording parameters as computed above and displays the various aberrations as a function of the wavelength in the form of a table. The performance of a conventional (mechanically ruled) grating with the same groove frequency is also shown in the same table for comparison.

SECTION 3. DATA SET AND DESCRIPTION OF DATA CARDS

This section discusses the input data required for a successful operation of the program.

(a) DATA SET

The following quantities are required as an input for this program:

1. λ_0 = the wavelength of recording laser light.

2. λ_1 = the lower limit of wavelength.

3. λ_2 = the upper limit of wavelength.

4. $\Delta\lambda$ = the wavelength interval selected for displaying the performance of the grating as a function of wavelength.

5. C = the angle 2κ (value 0.0 is used with option LMN = 2).

6. N = the number of lines per mm ($\sigma = 1/N$, the grating spacing in mm).

7. R = radius of curvature of the grating.

8. m = order of the diffraction where m takes on negative values for the program. m = -1, -2, etc.

9. IETA = parameter to specify the grating design method. (IETA = 1) specifies the General Method. (IETA = 0) specifies the Modified Method.

10. LMN = parameter to specify whether the angle 2κ is to be fed in as input (LMN = 1) or is to be computed by the optimization procedure (LMN = 2).

It should be noted "LMN" and "IETA" must be specified in the input for each data set for a successful run.

(b) DESCRIPTION OF DATA CARDS AND SAMPLE DATA CARD

The data set consists of ten parameters described in (a). The first seven parameters are to be punched in the order shown in (a), starting in column 1 in F10.0 format (i.e., ten columns are reserved for each of the six parameters and each of them must include a decimal).

The parameters m (-1, -2, -3, . . .), IETA (0,1) and LMN (1,2) take only single digit integer values. Two columns are therefore reserved for each of

(4) Operating Range = 0 Å to 4000 Å.

(5) Order m = -1.

(6) Determine the optimum angle 2κ.

Solution: (1) indicates that the modified method is used; IETA = 0. (6) indicates that the option LMN = 2 is to be used.

A data card is punched using the data supplied above and punched in the order listed below:

λ_0 = 4579.3

λ_1 = 0.0

λ_2 = 4000.0

$\Delta\lambda$ = 500.0

C = 0.0 (0.0 is punched on the input card when the optimum angle 2κ is to be determined)

N = 600.0

R = 1000.0

m = -1

IETA = 0

LMN = 2

Note that the wavelength input values are in angstroms, N in l/mm, and R in millimeters. The angle 2κ, where 2κ is C on the data card, is in degrees in decimal form.

The output data for the example cited is shown in Figure 5 and described as follows:

Line 1 shows the input parameters; order = -1 is the order of the grating, N = groove frequency in grooves per mm, R = radius of curvature of the grating in mm, IETA = 0 identifies the design method and LMN = 2 shows that the optimum angle 2κ has been calculated.

***** INPUT DATA *****

1 ORDER=-1 N= 600 GROOVES/MM RADIUS= 1000.0 MM TETA= 0 LMN= 2

2 LAMDAO= 4579.3 ANGST LAMDA1= 0.0 ANGST LAMDA2= 4000.0 ANGST

3 *****THE INSTRUMENTAL PARAMETERS*****

4 C=70.27/774 DEG RHOA=0.12231615D 01 RHOB=0.12245278D 01 SMLR=0.81755355D 03 MM SMPRP=0.81797731D 03 MM

5 ....ASTG TYPE ABBERATIONS MINIMISED......

6 *****RECORDING PARAMETERS******

7 GAMA=-.67513870D 02 DLTA=-.40482378D 02 RHOC=0.22490871D 01 RHOD=0.12223103D 01

8

9 / 10	LAMDA (ANGST)	F200 XF-04	F020	F300	F120	F400	F220	F040
MOD. METHOD	0.0	-0.082426	0.810167	0.000298	0.000594	0.810151	1.612818	0.408847
MECH. RULED		-0.082426	0.810167	0.000298	0.000594	0.810151	1.612818	0.408847
MOD. METHOD	500.0	0.001702	0.657043	0.007651	0.354405	0.741028	-0.256506	1.082392
MECH. RULED		0.001705	0.810442	0.015151	-0.029130	0.807958	1.614929	0.408599
MOD. METHOD	1000.0	0.037968	0.504469	0.014959	0.708201	0.667558	-2.121458	1.755397
MECH. RULED		0.037974	0.811268	0.029959	-0.058869	0.801417	1.621412	0.407810
MOD. METHOD	1500.0	0.034615	0.352447	0.022176	1.061966	0.589789	-3.982043	2.427859
MECH. RULED		0.034624	0.812645	0.044676	-0.088639	0.790578	1.632261	0.406478
MOD. METHOD	2000.0	0.005500	0.200978	0.029258	1.415686	0.507803	-5.838271	3.099776
MECH. RULED		0.005511	0.814575	0.059258	-0.118455	0.775522	1.647469	0.404602
MOD. METHOD	2500.0	-0.029835	0.050063	0.036160	1.769344	0.421714	-7.690153	3.771144
MECH. RULED		-0.029821	0.817060	0.073660	-0.148331	0.756362	1.667022	0.402176
MOD. METHOD	3000.0	-0.046060	-0.100294	0.042837	2.122926	0.331666	-9.537705	4.441957
MECH. RULED		-0.046043	0.820102	0.087837	-0.178285	0.733244	1.690904	0.399197
MOD. METHOD	3500.0	-0.011926	-0.250090	0.049245	2.476415	0.237838	-11.380947	5.112211
MECH. RULED		-0.011906	0.823705	0.101745	-0.208331	0.706346	1.719096	0.395657
MOD. METHOD	4000.0	0.109896	-0.399323	0.055336	2.829795	0.140441	-13.219903	5.781897
MECH. RULED		0.109918	0.827872	0.115336	-0.238486	0.675879	1.751575	0.391549

11 ....COMA TYPE ABBERATIONS MINIMISED......

12 *****RECORDING PARAMETERS******

13 GAMA=-.46056858D 02 DLTA=-.26440665D 02 RHOC=0.10469379D 01 RHOD=0.88010949D 00

14

15 / 16	LAMDA (ANGST)	F200 XF-04	F020	F300	F120	F400	F220	F040
MOD. METHOD	0.0	-0.082426	0.810167	0.000298	0.000594	0.810151	1.612818	0.408847
MECH. RULED		-0.082426	0.810167	0.000298	0.000594	0.810151	1.612818	0.408847
MOD. METHOD	500.0	0.001702	0.770231	0.007651	0.000578	0.802774	1.522464	0.382609
MECH. RULED		0.001705	0.810442	0.015151	-0.029130	0.807958	1.614929	0.408599
MOD. METHOD	1000.0	0.037968	0.730845	0.014959	0.000547	0.791049	1.436483	0.355830
MECH. RULED		0.037974	0.811268	0.029959	-0.058869	0.801417	1.621412	0.407810
MOD. METHOD	1500.0	0.034615	0.692011	0.022176	0.000486	0.775026	1.354868	0.328508
MECH. RULED		0.034624	0.812645	0.044576	-0.088639	0.790578	1.632261	0.406478
MOD. METHOD	2000.0	0.005500	0.653729	0.029258	0.000379	0.754786	1.277611	0.300642
MECH. RULED		0.005511	0.814575	0.059258	-0.118455	0.775522	1.647469	0.404602
MOD. METHOD	2500.0	-0.029835	0.616003	0.036160	0.000210	0.730442	1.204700	0.272226
MECH. RULED		-0.029821	0.817060	0.073660	-0.148331	0.756362	1.667022	0.402176
MOD. METHOD	3000.0	-0.046060	0.578834	0.042837	-0.000035	0.702140	1.136118	0.243256
MECH. RULED		-0.046043	0.820102	0.087837	-0.178285	0.733244	1.690904	0.399197
MOD. METHOD	3500.0	-0.011926	0.542275	0.049245	-0.000373	0.670058	1.071846	0.213727
MECH. RULED		-0.011906	0.823705	0.101745	-0.208331	0.706346	1.719096	0.395657
MOD. METHOD	4000.0	0.109896	0.506180	0.055336	-0.000820	0.634407	1.011860	0.183629
MECH. RULED		0.109918	0.827872	0.115336	-0.238486	0.675879	1.751575	0.391549

Figure 5

Line 2 shows the input values for λ_0 = LAMDA0 (laser wavelength), λ_1 = LAMDA1 (the lower wavelength limit), and λ_2 = LAMDA2 (upper wavelength limit).

Line 3 is self-explanatory.

Line 4 shows the calculated instrumental parameters; $C = 2\kappa$, $\bar{\rho}$ = RHOA, $\bar{\rho}'$ = RHOB, r_0' = SMLR in mm, and $\bar{r}_0'$ = SMPRP in mm. These parameters are defined in the text.

Line 5 shows the type of aberration that has been minimized: Astigmatism = ASTG.

Line 6 is self-explanatory and refers to line 7.

Line 7 shows the optimum recording parameters; γ = GAMA, δ = DLTA, ρ_C = RHOC and ρ_D = RHOD. These parameters have also been defined in the text.

Line 8 shows the titles for the table showing the performance of the grating as a function of wavelength. The table also shows the comparison of the holographic grating with the conventional grating having the same instrumental parameters.

λ = LAMDA is the wavelength at which the grating is evaluated.

$F_{200} \times 10^{-4}$ is the horizontal focus and astigmatism of the first term.

F_{020} is the vertical focus and astigmatism of the second term.

F_{300} is the first coma term.

F_{120} is the second coma term.

F_{400} is the first spherical aberration term.

F_{220} is the second spherical aberration term.

F_{040} is the third spherical aberration term.

Line 9 shows the holographic grating performance (Modified Method), the value of the wavelength and the values of the aberrations.

Line 10 shows the performance of a conventionally ruled grating (MECH. RULED).

Line 11 shows that the following information refers to minimizing coma type aberrations for the same instrumental parameters shown in Line 4.

Line 12 is self-explanatory and refers to Line 13.

Line 13 shows the recording parameters γ = GAMA, δ = DLTA, ρ_C = RHOC and ρ_D = RHOD required to fabricate a grating to minimize coma.

Lines 14, 15, and 16 are defined in the same way as Lines 8, 9, and 10 above. The values in this table refer to a grating designed to minimize coma over the desired wavelength.

REFERENCES

1. H. Greiner and E. Schaeffer, Optik <u>16</u>, 350 (1959)

2. H. Noda, T. Namioka and M. Seya, J. Optical Society of America <u>64</u>, 1043 (1974)

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COMPUTER PROGRAM FOR DESIGNING HOLOGRAPHIC GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

Part II: Correcting Aberrations at Specified Wavelengths

COMPUTER PROGRAM FOR DESIGNING HOLOGRAPHIC GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

PART II: CORRECTING ABERRATIONS AT SPECIFIED WAVELENGTHS

INTRODUCTION

A computer program has been developed based on the theory presented in papers by Greiner and Schaeffer (1) and Noda, Namioka, and Seya (2), that determines the optimum holographic grating recording parameters as a function of optical instrumental parameters and desired wavelength range for Seya-Namioka type monochromator mountings. In the first report, Part I, the holographic grating recording parameters are determined such that astigmatism or coma may be minimized over a selected wavelength range. In this report, Part II, we determine optimum recording parameters such that astigmatism or coma may be corrected at specified wavelengths. By corrected, we mean that the aberrations, astigmatism or coma, are zero at specified wavelengths. The program also simultaneously displays the performance of the holographic grating and equivalent conventional grating as a function of wavelength relative to optical aberrations of astigmatism, coma, and spherical aberration. In this report, two methods of designing holographic gratings for operation in negative orders only have been developed. The first method is the general method, and with this method the instrumental constants are related only to the holographic grating. The second method is the modified method and with this method it is possible to design holographic gratings that correct astigmatism or coma at specified wavelengths within the desired wavelength range for Seya-Namioka monochromators that are interchangeable with conventional gratings. This means that the instrumental constants are the same for both holographic gratings and conventional gratings.

The contents of this report is divided into four sections. Section I presents the theory and basic equations for designing holographic concave gratings such that correction for aberrations of astigmatism or coma at a specified wavelength may be achieved. The basic equations are extracted from Ref. 2 and are presented so that a better understanding of the computer program may be appreciated. However, we have modified the equations for minimizing astigmatism or coma such that they will now correct astigmatism or coma at specified wavelengths λ^*. A description of the computer program including all of the subroutines is presented in Section 2. Section 3 presents the input data, definition of terms, and data card description. Section 4 presents an example for using the program and also describes the output data in detail.

SECTION I. Theory and Basic Equations for Designing Holographic Concave Gratings.

Since a detailed theoretical explanation relative to the design of holographic concave gratings is given in Ref. 2 we only present a brief description for ease of understanding the development of the computer program presented in this report.

Figure 1 shows a schematic diagram of the optical system which defines a rectangular coordinate system. We have used the same terminology as Noda, Namioka, and Seya (Ref. 2) in order to avoid any ambiguity. Let the origin be at vertex 0 of the concave grating having a radius of curvature R. Let the x-axis be the normal to the grating at 0 and let the xy plane be defined by 0 and two coherent point sources C and D used to record the interference fringes on a concave substrate. Points A, P, and B are self luminous points on the entrance slit, a point on the grating and a point at the focus on the diffracted image from P of wavelength in the m^{th} order, respectively.

For the ray APB, the light path function F is given by

$$F = F_{000} + wF_{100} + lF_{011} + \frac{1}{2}w^2F_{200} + \frac{1}{2}l^2F_{020} + \frac{1}{2}w^2F_{300}$$

$$+ \frac{1}{2}wl^2F_{120} + wlF_{111} + \frac{1}{8}w^4F_{400} + \frac{1}{4}w^2l^2F_{220} + \frac{1}{8}l^4F_{040}$$

$$+ \frac{1}{4}w^2F_{202} + \frac{1}{4}l^2F_{022} + \frac{1}{2}l^3F_{031} + \frac{1}{2}w^2lF_{211} + \cdots \tag{1}$$

and

$$F_{ijk} = M_{ijk} + (m\lambda/\lambda_0)H_{ijk}, \tag{2}$$

The M terms refer to the contribution of the conventionally rulled grating and the H terms refer to the contribution of the holographic grating. In Eq. 2, m is the order of the grating, λ_0 is the laser radiation wavelength and λ is the wavelength at which the grating is being employed. The terms Mijk and Hijk are defined in terms of the functions fijk as follows:

$$M_{ijk} = f_{ijk}(\rho, \alpha) + f_{ijk}(\rho', \beta),$$

$$H_{ijk} = f_{ijk}(\rho c, \gamma) - f_{ijk}(\rho D, \delta) \tag{3}$$

for

$$(ijk) = (200),\ (020),\ (300),\ (120),$$

$$M_{ijk} = M_{020} - (-1)^{\frac{1}{2}i}[f_{ijk}(\rho,\alpha) + f_{ijk}(\rho',\beta)],$$

$$H_{ijk} = H_{020} - (-1)^{\frac{1}{2}i}[f_{ijk}(\rho_C,\gamma) - f_{ijk}(\rho_D,\delta)] \tag{4}$$

for

$$(ijk) = (400),\ (220),\ (040),$$

where

$$f_{200}(\rho,\alpha) = (\rho\cos\alpha - 1)\cos\alpha,$$

$$f_{020}(\rho,\alpha) = \rho - \cos\alpha,$$

$$f_{300}(\rho,\alpha) = \rho\sin\alpha \cdot f_{200}(\rho,\alpha),$$

$$f_{120}(\rho,\alpha) = \rho\sin\alpha \cdot f_{020}(\rho,\alpha),$$

$$f_{400}(\rho,\alpha) = \rho f_{200}(\rho,\alpha)\ [f_{200}(\rho,\alpha) - 4\rho\sin^2\alpha],$$

$$f_{220}(\rho,\alpha) = \rho f_{020}(\rho,\alpha)\ [2\rho\sin^2\alpha - f_{200}(\rho,\alpha)],$$

$$f_{040}(\rho,\alpha) = \rho[f_{020}(\rho,\alpha)]^2 \tag{5}$$

$$\rho = R/r, \qquad \rho' = R/r', \qquad \rho_C = R/r_C, \qquad \rho_D = R/r_D, \tag{6}$$

$$x = r\cos\alpha, \qquad y' = r\sin\alpha, \qquad x' = r'\cos\beta, \qquad y' = r'\sin\beta,$$

$$x_C = r_C\cos\gamma, \qquad y_C = r_C\sin\gamma, \qquad x_D = r_D\cos\delta, \qquad y_D = r_D\sin\delta. \tag{7}$$

For equations (2)-(7), R is the radius of curvature of the grating and (r_C, γ, 0) and (r_D, δ, 0) are respectively the cylindrical coordinates of the point sources C and D.

The grating equation is given by

$$\sigma(\sin\alpha_0 + \sin\beta_0) = m\lambda \tag{8}$$

for the principal ray, the ray originating from the center of the entrance slit, and diffracted from 0 at an angle β. σ is the effective grating constant defined by

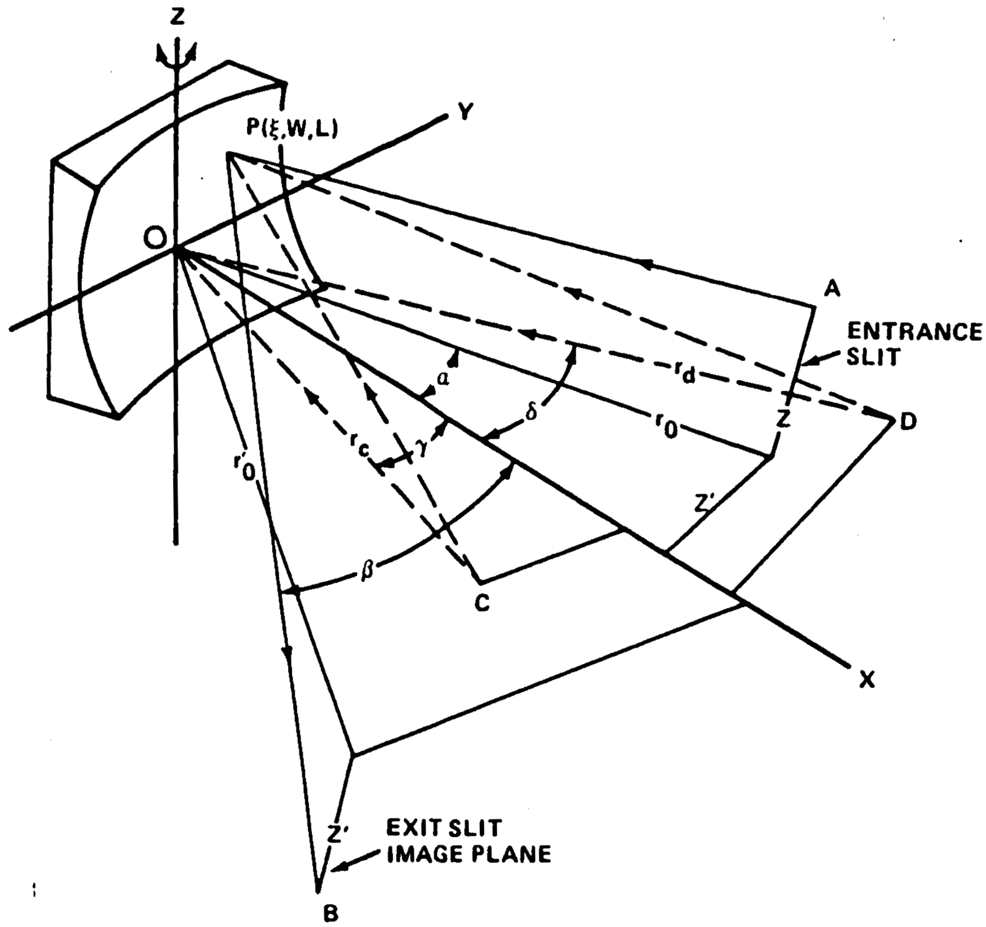


Figure 1. Schematic diagram showing the geometry for recording holographic gratings. The instrumental and recording parameters are defined as follows:

(Instrumental Parameters):

r_0 is the objective distance from the entrance slit to the center of the grating.

r'_0 is the image distance from the exit slit to the center of the grating.

α is the angle of incident radiation relative to the normal of the grating.

β is the diffracted image angle relative to the normal of the grating.

A is the entrance slit position and B is the exit slit position.

(Recording Parameters):

r_c is the distance of recording point source C to the center of the grating.

r_d is the distance of the recording point source D to the center of the grating.

δ is the recording angle for positioning point source D relative to the normal of the grating.

γ is the recording angle for positioning point source C relative to the normal of the grating.

$$\sigma = \frac{\lambda_0}{\sin\delta - \sin\gamma}$$

where

$$\delta > \gamma$$

Note that the number of grooves per unit length is $N = 1/\sigma$.

Minimization of Aberration Terms

The theory described up to this point has been presented for the general case. We now apply the general theory to a specific application; the Seya-Namioka monochromator. For the Seya-Namioka monochromat the basic instrumental parameters are defined as follows; (reference 2) see Figure 2.

$$r_0,\ \bar{r}'_0 = \text{constant}, \qquad 2K = \alpha_0 - \beta_0 = \text{constant}$$

$$\alpha_0 = K + \theta, \qquad \beta_0 = \theta - K \tag{10}$$

where r_0 is the distance from the center of the entrance slit to 0 and $\bar{r}'_0$ is the distance from 0 to the center of the exit slit. 2K is the angle AOB and θ is the angle of grating rotation measured from the bisector of the angle 2K and has the same sign as the spectral order m. Under conditions (10), the relation between θ and λ is given by

$$\lambda = \frac{2\sigma}{m} \cos K \sin\theta \tag{11}$$

We denote F_{ijk} for the ray AOB by $\bar{F}_{ijk}$. Then, the aberrations in the Seya-Namioka monochromator can be reduced by minimizing the functions

$$\bar{F}_{ijk}(\bar{\rho}, \bar{\rho}', \theta, K, A_{ijk}) = \bar{M}_{ijk} + \frac{m\lambda}{\lambda_0} H_{ijk}$$

$$= \bar{M}_{ijk} + A_{ijk}(\sin\alpha_0 + \sin\beta_0) \tag{12}$$

where

$$i + J + K \geqq 2$$

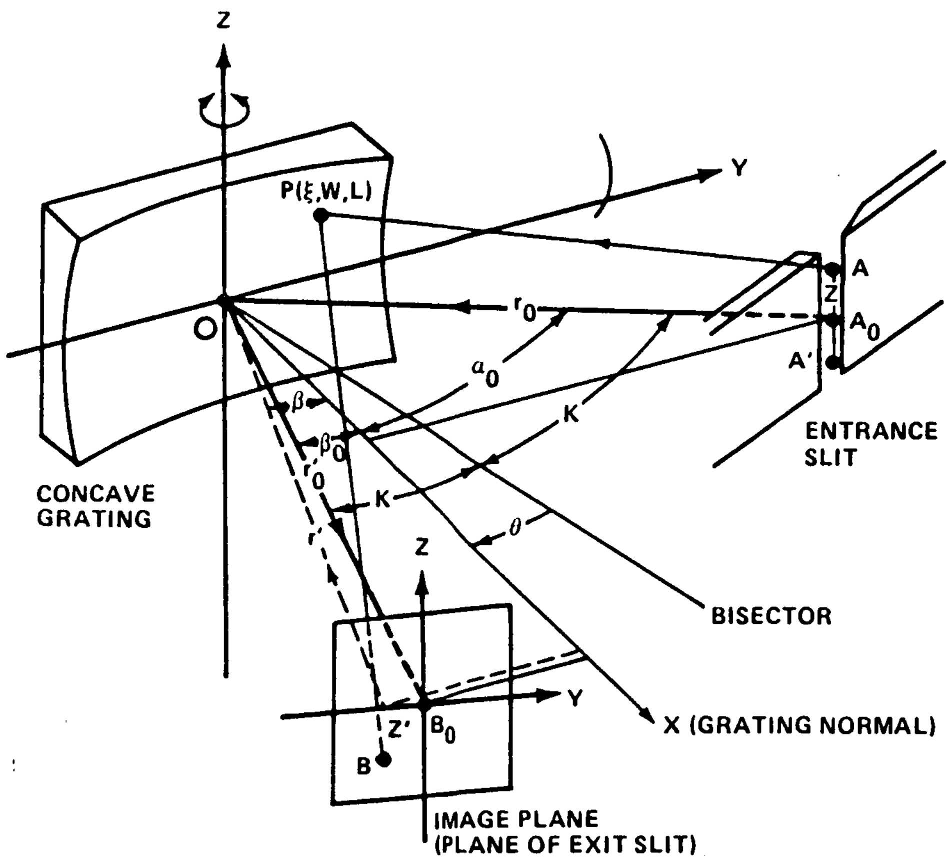


Figure 2. Schematic diagram of the optical system for Seya-Namioka monochromator

over a predetermined scanning range, $\theta_1 \leqq \theta \leqq \theta_2$ or $\lambda_1 \leqq \lambda \leqq \lambda_2$ where

$$\overline{\rho} = \frac{R}{r_0}, \; \overline{\rho}' = \frac{R}{\overline{r}'} = \frac{R}{r_0'}, \tag{13}$$

$$A_{ijk} = \frac{H_{ijk}}{\sin\delta - \sin\gamma} = \left(\frac{\sigma}{\lambda_0}\right) H_{ijk} \tag{14}$$

and θ_1, and θ_2 are related to λ_1 and λ_2 through equation (11). This is equivalent to imposing on $\overline{F}_{ijk}$'s the condition

$$I_{ijk} \equiv \int_{\theta_1}^{\theta_2} \overline{F}^2_{ijk}\, d\theta = \text{minimum} \tag{15}$$

Determination of Instrumental Parameters $\overline{\rho}$, $\overline{\rho}'$, K and A_{200}

The optimum instrumental parameters are determined in such a way that Eq. (15) is satisfied for the horizontal focusing condition $\overline{F}_{200}$. This is accomplished by solving the following equations simultaneously,

$$\frac{\partial I_{200}}{\partial \overline{\rho}} = 0, \qquad \frac{\partial I_{200}}{\partial \overline{\rho}'} = 0,$$

$$\frac{\partial I_{200}}{\partial K} = 0, \qquad \frac{\partial I_{200}}{\partial A_{200}} = 0. \tag{16}$$

Once the optimum values of $\overline{\rho}$, $\overline{\rho}'$ and K are determined, then each one of the integrals I_{ijk} with $i + J + K \geqq 2$ becomes a function only of A_{ijk}. Then, those values of A_{ijk}'s which satisfy Eq. (15) are calculated from the equation

$$\frac{\partial I_{ijk}}{\partial A_{ijk}} = 0:$$

where

$$A_{ijk} = [B_{ijk}(\theta_2) - B_{ijk}(\theta_1)] /$$

$$[2(\theta_2 - \theta_1) - (\sin 2\theta_2 - \sin 2\theta_1)] \cos K, \tag{17}$$

where

$$B_{200}(\theta) = (\bar{\rho}/3)\ [\cos\theta + \cos(\theta + K)\cos(2\theta + K$$

$$+ 3\sin(\theta + K)\sin K]$$

$$+ (\bar{\rho}'/3)\ [\cos\theta + \cos(\theta - K)\cos(2\theta - K)$$

$$- 3\sin(\theta - K)\sin K] - \cos 2\theta \cos K, \tag{18}$$

$$B_{020}(\theta) = 2(\bar{\rho} + \bar{\rho}')\cos\theta - \cos 2\theta \cos K, \tag{19}$$

$$B_{300}(\theta) = (\bar{\rho}/4)^2\ [\sin(4\theta + 3K)$$

$$- 4\cos 2(\theta + K)\sin K - 4\theta \cos K]$$

$$+ (\bar{\rho}'/4)^2\ [\sin(4\theta - 3K)$$

$$+ 4\cos(\theta - K)\sin K - 4\theta\cos K]$$

$$+ (\bar{\rho}/6)\ [3\sin(\theta + 2K) - \sin(3\theta + 2K)]$$

$$+ (\bar{\rho}'/6)\ [3\sin(\theta - 2K) - \sin(3\theta - 2K)], \tag{20}$$

$$B_{120}(\theta) = \frac{1}{2}\bar{\rho}^2[\sin(2\theta + K) - 2\theta\cos K]$$

$$+ \frac{1}{2}\bar{\rho}'^2\ [\sin(2\theta - K) - 2\theta\cos K]$$

$$+ (\bar{\rho}/6)\ [3\sin(\theta + 2K) - \sin(3\theta + 2K)]$$

$$+ (\bar{\rho}'/6)\ [3\sin(\theta - 2K) - \sin(3\theta - 2K)], \tag{21}$$

and so on.

Determination of the Recording Parameters ρ_c, ρ_D, γ and δ to Correct for Astigmatism or Coma at a Specified Wavelength

The recording parameters are dependent upon the aberrations to be corrected and the selected correcting wavelength λ^*. With a predetermined effective grating constant, the following equations are solved simultaneously for correcting astigmatism and one coma type aberration,

$$\left.\begin{aligned}
&\sin\delta - \sin\gamma = N\lambda_0\\
&f_{200}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = N\lambda_0 A_{200}\\
&f_{300}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = -\frac{\lambda_0}{m\lambda^*}\,[\bar{\rho}\sin\alpha^*(\bar{\rho}\cos^2\alpha^* - \cos\alpha^*)\\
&\qquad\qquad + \bar{\rho}'\sin\beta^*(\bar{\rho}'\cos^2\beta^* - \cos\beta^*)]\\
&f_{020}(\rho_c, \gamma) - f_{020}(\rho_D, \delta) = -\frac{\lambda_0}{m\lambda^*}\,[\bar{\rho} + \bar{\rho}' - (\cos\alpha^* + \cos\beta^*)]
\end{aligned}\right\} \quad (22)$$

and for correcting coma-type aberrations

$$\left.\begin{aligned}
&\sin\delta - \sin\gamma = N\lambda_0\\
&f_{200}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = N\lambda_0 A_{200}\\
&f_{300}(\rho_c, \gamma) - f_{300}(\rho_D, \delta) = -\frac{\lambda_0}{m\lambda^*}\,[\bar{\rho}\sin\alpha^*(\bar{\rho}\cos^2\alpha^* - \cos\alpha^*)\\
&\qquad\qquad + \bar{\rho}'\sin\beta^*(\bar{\rho}'\cos^2\beta^* - \cos\beta^*)]\\
&f_{120}(\rho_c, \gamma) - f_{120}(\rho_D, \delta) = -\frac{\lambda_0}{m\lambda^*}\,[\bar{\rho}\sin\alpha^*(\bar{\rho} - \cos\alpha^*)\\
&\qquad\qquad + \bar{\rho}'\sin\beta^*(\bar{\rho}' - \cos\beta^*)]
\end{aligned}\right\} \quad (23)$$

Before making any attempt to solve Equations (22) or (23) it is necessary to investigate the conditions under which Equations (22) or (23) can have real solutions for ρ_c and ρ_D because H_{300} and H_{120} are quadratic in ρ_c and ρ_D and their values depend on A_{300} and A_{120} and therefore on values of θ_2 in I_{300} and I_{120}. The condition may be stated in such a way that two quadratic equations of ρ_c or

ρ_D resulting from equations (22) and (23) should not have imaginary roots. To fulfill this condition, A_{300} must satisfy the equation

$$b^2 - 4ac \geqq 0 \tag{24}$$

where for A_{300}

$$a = (\sin\delta \cos^2\gamma - \sin\gamma \cos^2\delta) \cos^2\gamma,$$

$$b = [2p \cos\gamma \sin\delta + \sin(\delta - \gamma) \cos\delta] \cos\gamma,$$

$$c = p(p + \cos\delta) \sin\delta + A_{200} \cos^2\delta (\sin\delta - \sin\gamma), \tag{25}$$

$$p = A_{200}(\sin\delta - \sin\gamma) + \cos\gamma - \cos\delta. \tag{26}$$

When condition (24) is satisfied, then ρ_c and ρ_D are solutions to Equations 22 and 23. Up to this point, we have been describing the general method of designing aberration corrected holographic gratings for Seya-Namioka monochromators which are not interchangeable with conventional gratings. The next paragraph describes the method where the conventional and holographic gratings are interchangeable.

Modified Method

The modified method of designing holographic gratings for the Seya-Namioka monochromator has a practical advantage in that the holographic grating is interchangeable with a conventionally ruled grating having the same radius of curvature.

This is possible provided the same instrumental constants $\bar{\rho}$, $\bar{\rho}'$ and K used for the conventionally ruled grating are used to design the holographic grating. The instrumental constants for the conventional grating are determined by solving the equation

$$I_{200} \equiv \int_{\theta_1}^{\theta_2} \bar{M}_{200}^2 \, d\theta = \text{minimum}.$$

or

$$\frac{\partial I_{200}}{\partial \bar{\rho}} = 0, \qquad \frac{\partial I_{200}}{\partial \bar{\rho}'} = 0$$

and

$$\frac{\partial I_{200}}{\partial K} = 0. \tag{27}$$

The design procedure given by Equations (15)-(23) must be modified in part in order to accommodate condition (27). The modification required is to replace Eq. (16) with Equation (27) and Equation (17) with $(ijk) = (200)$ and the rest of the procedure remains the same.

SECTION 2

Section 1 described the theory for designing holographic gratings that correct astigmatism or coma at specified wavelengths within a desired wavelength range. In this section, we use the theory and present the computer program which consists of a main program and four subroutines. Figure (3) is a diagram of the flow chart for the program.

PROGRAM DESCRIPTION

The following is a presentation of the main program and algorithms for each subroutine in the computer program to show how the algorithms perform their specific tasks.

MAIN PROGRAM

The purpose of this program is to direct the flow of calculations depending upon which option is selected. If option LMN = 2 is selected, then the optimum value of the instrumental parameter angle 2K will be calculated. However, if the programmer chooses to specify an angle 2K as an input value, then option LMN = 1 is used.

The computer program has been developed to accommodate two holographic grating design methods; the general method and the modified method. If the general method is selected, then the option called IETA = 1 is used in the program. When using option IETA = 1, all the instrumental parameters are related only to the holographic grating.

If the modified method is selected, then option IETA = 0 is used in the program. When using this option, all calculated instrumental parameters are the same for both holographic and conventional gratings. This means that the holographic and conventional gratings are interchangeable if they have the same groove frequency and radius of curvature. The only difference is that the holographic grating corrects aberrations to zero and the conventional grating does not.

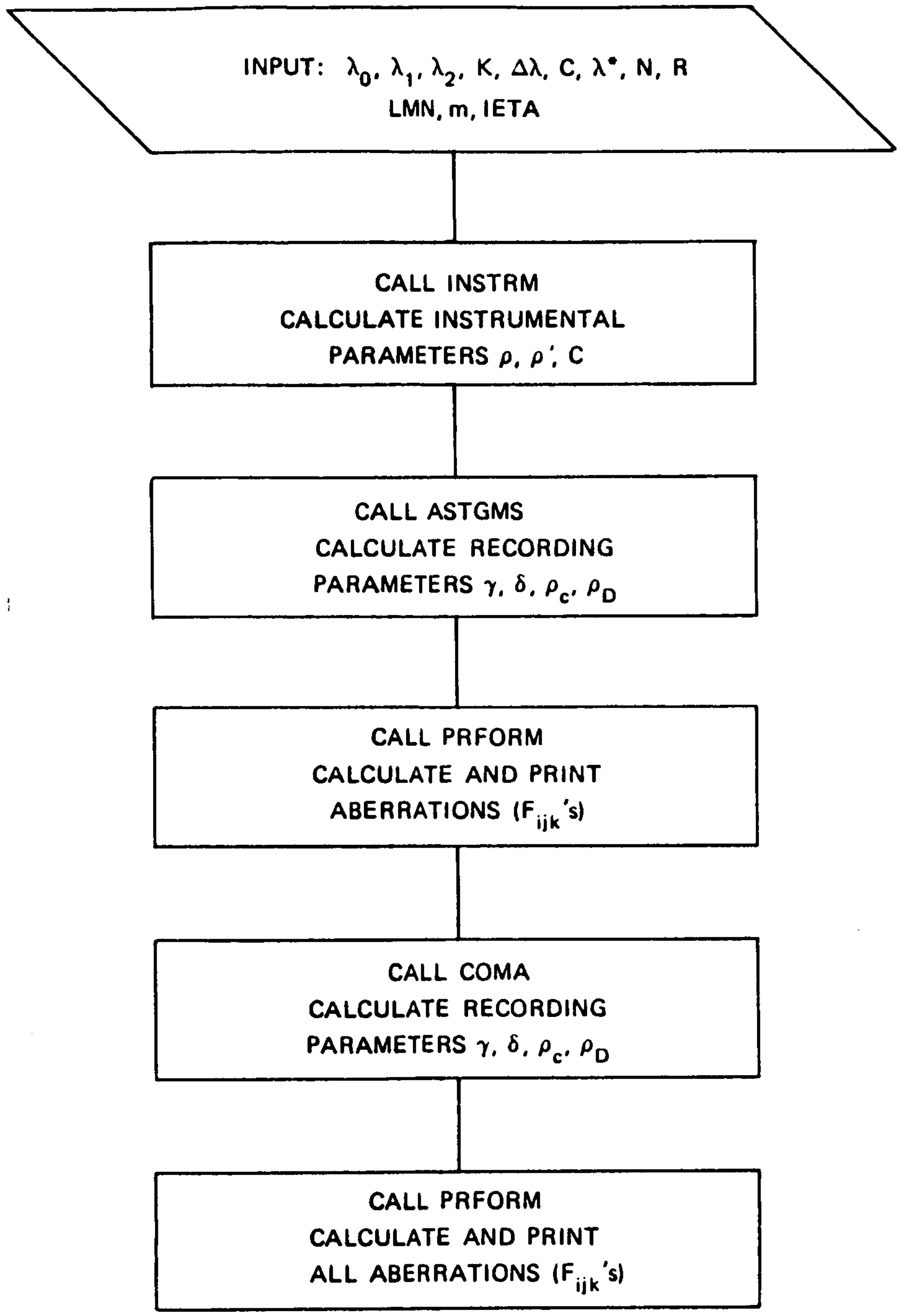


Figure 3. Main Program Flow Chart

Once the design method has been selected and the LMN option has been chosen, the following steps of calculation are performed.

STEP A: Read input cards.

STEP B: Call INSTRM to calculate the optimum angle 2K, and then calculate Bijk and Aijk Eqs. (17) (LMN 2) or calculate the functions Bijk and Aijk using the input value of 2K (LMN = 1).

STEP C: Call ASTGMS to calculate the recording parameters ρ_c, ρ_D, γ, and δ to correct astigmatism ijk = (020) and one coma term ijk = (300) at λ^*.

STEP D: Call COMA to calculate the recording parameters ρ_c, ρ_D, γ, δ to correct coma aberrations (ijk) = (300) and (ijk) = (120) at λ^*.

STEP E: Call PRFORM to display the numerical values of each aberration for the holographic grating and compare with that of the equivalent conventional grating as a function of wavelength. Note that the program automatically calculates the recording parameters for both the astigmatism correction and coma correction. This feature was included in the program so that the program user may select which aberration correction will best produce the optimum performance for all aberrations (astigmatism, coma and spherical) throughout the desired wavelength range.

Subroutine INSTRM

This subroutine obtains the optimum values of the instrumental parameters namely $\bar{\rho}$, $\bar{\rho}'$, 2K and A200 by simultaneous solution of Eqs. (16). A modified form of Newton's method is used to obtain the solution. The quantities Bijk's are then calculated using the optimum values of $\bar{\rho}$, $\bar{\rho}'$ and 2K which in turn give A_{ijk} by Eq. (17). If a prescribed input value of 2K were used, the selection of option LMN = 1 would by-pass the optimization procedure when calculating the other instrumental parameters.

The values of the instrumental parameters as well as A_{300}, A_{020}, and A_{120} are printed at the end of this subroutine.

Subroutine ASTGMS

The purpose of this subroutine is to obtain the recording parameters such that astigmatism (ijk) = (020) and a coma type term (ijk) = (300) are corrected for a specified wavelength λ^*. This is achieved by finding a simultaneous solution of Eq. (22).

It is first verified that the quantity $N\lambda_0$ is less than the maximum value of $|(\sin\delta - \sin\gamma)|$; namely 2. If not, an error message is printed stating "error, gamma out of bounds."

The values of a, b, c of Eqs. (25) are then computed and the discriminant is checked to ensure $b^2 - 4ac \geq 0$. The solutions of the quadratic equation are computed and checked for positiveness; the calculation shows that one of the two roots $[-b + \sqrt{b^2 - 4ac}/2a]$ is always positive and the other always negative.

The value of the angle γ to the desired accuracy is determined by the iterated solution of Eq. (22) by Newton's method. The resulting values of the recording parameters γ and δ are printed at the end of this subroutine.

Subroutine COMA

The purpose of this subroutine is to obtain the recording parameters such that the coma type terms (ijk) = (300) and (120) are corrected at a specified wavelength λ^*.

It is first verified that the quantity $N\lambda_0$ is less than the maximum value of $|(\sin\delta - \sin\gamma)|$; namely 2. If not, an error message is printed stating "error, gamma out of bounds."

The value of a, b, c of Eq. (25) are then computed and the discriminant is checked to ensure that $b^2 - 4ac \geq 0$. The solutions of the quadratic equation are computed and verified for positiveness; the calculation shows that one of the two roots $[-b + \sqrt{b^2 - 4ac}/2a]$ is always positive and the other always negative.

The value of the angle γ to the desired accuracy is determined by the iterated solution of Eq. (22) by Newton's method. The resulting values of the recording parameters γ and δ are printed at the end of this subroutine.

Subroutine PRFORM

This subroutine calculates the performance of the holographic grating with the recording parameters as computed above and displays the various aberrations as a function of the wavelength in the form of a table. The performance of an equivalent conventional (mechanically ruled) grating with the same groove frequency is also shown in the same table for comparison.

SECTION 3. DATA SET AND DESCRIPTION OF DATA CARDS

This section discusses the input data required for successful operation of the program.

(a) DATA SET

The following quantities are required as input data for this program:

(1) λ_0 = wavelength of laser recording radiation.

(2) λ_1 = lower wavelength limit.

(3) λ_2 = upper wavelength limit.

(4) $\Delta\lambda$ = wavelength interval at which aberrations will be displayed.

(5) λ^* = wavelength at which aberrations will be corrected.

(6) C = angle 2K (value 0.0 is used with option LMN = 2).

(7) N = number of lines per mm. ($\sigma = 1/N$; grating spacing).

(8) R = radius of curvature of the grating in mm.

(9) LMN = Parameter to specify whether the angle 2K is to be fed in as an input (LMN = 1) or is to be computed by the optimization procedure (LMN = 2).

(10) m = order of diffraction where m takes on negative values.

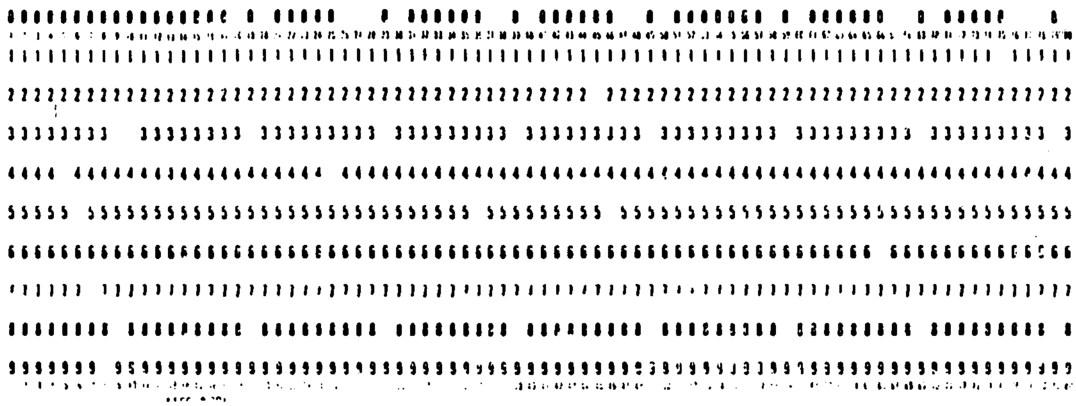
(11) IETA = Parameter to specify the grating design method:
(IETA = 1) specifies the general method
(IETA = 0) specifies the modified method.

Note that "LMN" and "IETA" must be specified in the input for each data set for a successful run.

(b) DESCRIPTION OF DATA CARDS AND SAMPLE DATA CARDS

The data set consists of eleven parameters described in (a). The first eight parameters are punched on the first card in the order stated in (a) starting in column 1 in F10.0 format. For example, ten columns are reserved for each of the eight parameters and each must include a decimal. The parameters LMN (1,2), m(-1, -2, ...) and IETA (0, 1) are punched on the second card using only single digit integer values and two columns are reserved for each of these parameters starting in column 1. Figure 4 illustrates typical data cards with the input values shown at the top.

4579.3	0.0	4000.0	500.0	2500.0	0.0	600.0	1000.0
λ_0	λ_1	λ_2	$\Delta\lambda$	λ^*	C	N	R



2–1 1
LMN M IETA

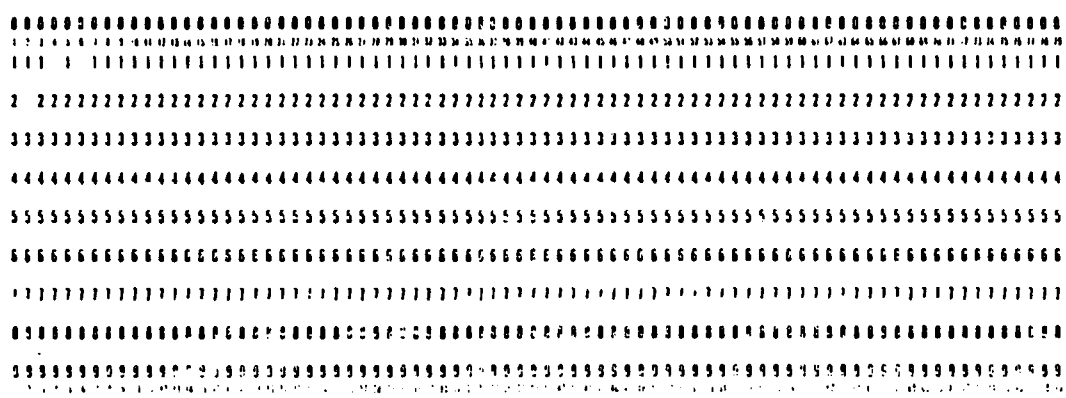


Figure 4

Note that as many data sets as desired may be put into a single program run provided that the values of all eleven parameters are punched for each data set which consists of two cards.

SECTION 4

This section presents a typical example for using the program and also describes the output data in detail.

Example: Determine the optimum instrumental and recording parameters for the design of a holographic grating that corrects astigmatism or coma to zero at 2500 A having the following specifications:

(1) Groove frequency = 600 l/mm
(2) Radius of curvature = 1000 mm
(3) Operating range = 0 A to 4000 A
(4) Order m = -1
(5) Determine the optimum angle 2K
(6) This holographic grating is not interchangeable with a conventional grating.

Solution: (5) indicates that the option LMN = 2 will be used. (6) specifies that the General Method of design will be used (IETA = 1). A data card is punched using the data supplied above and punched in the order listed below:

λ_0 = 4579.3
λ_1 = 0.0
λ_2 = 4000.0
$\Delta\lambda$ = 500.0
λ^* = 2500.0
C = 0.0 (0.0 is punched on the input card when the optimum angle 2K is to be determined).
N = 600.0
R = 1000.0
LMN = 2
m = -1
IETA = 1

Note that the wavelength input values are in angstroms, N in lines per mm and R in mm. The angle 2K, where 2K = C on the data card, is in degrees in decimal form.

The output data for the example cited is shown in Fig. 5 and described as follows:

Line 1; shows the input parameters; order = -1 is the order of the grating, N = groove frequency, R = radius of curvature of the grating, IETA = 1 identifies the design method, and LMN = 2 shows that the optimum angle 2K has been calculated.

Line 2; the input values for λ_0 = LAMDAO (laser wavelength), λ_1 = LAMDA1 (lower wavelength limit), λ_2 = LAMDA2 (upper wavelength limit) and λ^* = LAMDAC (correcting wavelength).

Line 3; is self explanatory.

Line 4; shows the calculated instrumental parameters C = 2K, $\bar{\rho}$ = RHOA, $\bar{\rho}'$ = RHOB, r_0' = SMLR in mm and $\bar{r}_0'$ = SMPRP in mm. These parameters are defined in the text.

Line 5; shows the type of aberration that has been corrected; Astigmatism = ASTG.

Line 6; is self explanatory and refers to line 7.

Line 7; shows the optimum recording parameters γ = GAMA, δ = DLTA, ρ_c = RHOC and ρ_D = RHOD. These parameters have also been defined in the text.

Line 8; shows the wavelength (λ = LAMDA) at which the grating is evaluated and the aberration terms described as follows:

$F_{200} \times 10^{-4}$ is the horizontal focus and astigmatism of the first term.

F_{020} is the vertical focus and astigmatism of the second term.

F_{300} is the first coma term.

F_{120} is the second coma term.

F_{400} is the first spherical aberration term.

F_{220} is the second spherical aberration term.

F_{040} is the third spherical aberration term.

Line 9; shows the holographic grating performance (General Method), the evaluating wavelength and the values of the aberrations.

Line 10; shows the performance of the equivalent conventional grating (MECH. RULED).

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***** INPUT DATA *****

Line 1 ORDER=-1 N= 600 GROOVES/MM RADIUS= 1000.0 MM IETA= 1 IMN= 2

2 LAMDAO= 4579.3 ANGST LAMDA1= 0.0 ANGST LAMDA2= 4000.0 ANGST LAMDAC= 2500.0 ANGST

3 ******THE INSTRUMENTAL PARAMETERS*****

4 C=70.264923 DEG RHOA=0.12230965D 01 RHOB=0.12224022D 01 SALH=0.41755669D 03 MM SHPRP=0.41305056D 03 MM

5 ....ASTG TYPE ABERRATIONS CORRECTED......

6 *****RECORDING PARAMETERS******

7 GAMA=-.55851322D 02 DLTA=-.36154682D 02 RHOC=0.27055520D 01 RHOD=0.18151259D 01

8 / 9 / 10

	LAMDA (ANGST)	F200 *E-04	F020	F300	F120	F400	F220	F040
GEN. METHOD	0.0	-0.056030	0.805853	0.000325	0.000650	0.403433	1.511921	0.409975
MECH. RULED		-0.056030	0.805853	0.000325	0.000650	0.373933	1.511821	0.409975
GEN. METHOD	500.0	-0.002457	0.846775	0.043647	0.464406	0.283199	-0.956591	1.597124
MECH. RULED		-0.002811	0.810126	0.015174	-0.029060	0.397641	1.513924	0.409629
GEN. METHOD	1000.0	0.039654	0.484257	0.011522	0.029147	-0.251793	-3.336514	2.785233
MECH. RULED		0.040026	0.810953	0.029571	-0.058736	0.371102	1.523357	0.407983
GEN. METHOD	1500.0	0.040153	0.322283	0.130167	1.152358	-0.733071	-6.104281	3.972400
MECH. RULED		0.040711	0.812330	0.044663	-0.088682	0.737264	1.531235	0.405515
GEN. METHOD	2000.0	0.012344	0.186664	0.173187	1.857521	-1.314563	-9.447592	5.159422
MECH. RULED		0.013087	0.814260	0.085253	-0.118343	0.775211	1.546427	0.404642
GEN. METHOD	2500.0	-0.024246	-0.300000	0.216027	2.321527	-1.841165	-11.226553	6.345996
MECH. RULED		-0.023317	0.816745	0.073086	-0.148206	0.754065	1.655567	0.402221
GEN. METHOD	3000.0	-0.044304	-0.168303	0.225677	2.785653	-2.411721	-13.781193	7.531416
MECH. RULED		-0.043185	0.815787	0.087824	-0.178146	0.712351	1.599833	0.392247
GEN. METHOD	3500.0	-0.016555	-0.320058	0.301047	3.249549	-2.515351	-15.331530	8.716577
MECH. RULED		-0.015258	0.822385	0.101722	-0.208179	0.735072	1.718007	0.395713
GEN. METHOD	4000.0	0.056178	-0.475230	0.242121	3.712411	-3.513951	-18.377575	9.901171
MECH. RULED		0.057665	0.827556	0.115311	-0.238320	0.675611	1.750465	0.391511

11 ....COMA TYPE ABERRATIONS CORRECTED......

12 *****RECORDING PARAMETERS******

13 GAMA=-.51831857D 02 DLTA=-.30843764D 02 RHOC=0.54167448D 00 RHOD=0.42432345D 00

14 / 15 / 16

	LAMDA (ANGST)	F200 *E-04	F020	F300	F120	F400	F220	F040
GEN. METHOD	0.0	-0.096030	0.805853	0.000325	0.000650	0.403433	1.511921	0.409975
MECH. RULED		-0.056030	0.805853	0.000325	0.000650	0.403833	1.511921	0.409875
GEN. METHOD	500.0	-0.002557	0.766564	0.004064	0.000551	0.310147	1.519519	0.377959
MECH. RULED		-0.002411	0.810126	0.015174	-0.029060	0.397641	1.513924	0.409629
GEN. METHOD	1000.0	0.035654	0.778666	0.011734	0.000497	0.305181	1.431567	0.349580
MECH. RULED		0.040026	0.810953	0.029573	-0.058786	0.381102	1.523357	0.407943
GEN. METHOD	1500.0	0.040153	0.788530	0.017371	0.000382	0.737597	1.347093	0.319121
MECH. RULED		0.040711	0.812330	0.044653	-0.088642	0.711253	1.531235	0.405515
GEN. METHOD	2000.0	0.012344	0.846666	0.022743	0.000222	0.743381	1.298773	0.289117
MECH. RULED		0.013087	0.814260	0.058253	-0.118343	0.775214	1.546429	0.404942
GEN. METHOD	2500.0	-0.024246	0.811027	0.020087	-0.000030	0.759773	1.193837	0.256565
MECH. RULED		-0.023317	0.816745	0.073054	-0.148206	0.755065	1.665967	0.402221
GEN. METHOD	3000.0	-0.044304	0.772526	0.033123	-0.000299	0.759203	1.123349	0.224455
MECH. RULED		-0.043185	0.815787	0.047824	-0.178146	0.712354	1.599833	0.392247
GEN. METHOD	3500.0	-0.016555	0.535385	0.037553	-0.000690	0.723851	1.757109	0.191794
MECH. RULED		-0.015758	0.822385	0.101725	-0.208179	0.734072	1.719007	0.395713
GEN. METHOD	4000.0	0.056178	0.456406	0.042271	-0.001195	0.615945	0.795154	0.159561
MECH. RULED		0.097665	0.827556	0.115311	-0.238320	0.673611	1.753465	0.391511

Figure 5

Line 11; shows that the following information refers to correcting coma type aberrations for the same instrumental parameters shown in line 4.

Line 12; is self explanatory and refers to line 13.

Line 13; shows the recording parameters γ = GAMA, δ = DLTA, ρ_c = RHOC, ρ_D = RHOD required to fabricate a grating to correct for coma.

Lines 14, 15 and 16 are defined in the same way as lines 8, 9, and 10 above. The values in this table refer to a grating designed to correct for coma at a specified wavelength. In this example the correcting wavelength is 2500A.

REFERENCES

(1) H. Greiner and E. Schaeffer, Optik 16, 350(1959)

(2) H. Noda, T. Namioka and M. Seya, J. Optical Society of America 64, 1043 (1974)

(3) T. Namioka, H. Noda and M. Seya, Science of Light. 22, 77(1973).

DESIGN OF ASTIGMATISM OR COMA CORRECTED HOLOGRAPHIC GRATINGS FOR ROWLAND CIRCLE SPECTROGRAPHIC MOUNTS

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DESIGN OF ASTIGMATISM OR COMA CORRECTED HOLOGRAPHIC GRATINGS FOR ROWLAND CIRCLE SPECTROGRAPHIC MOUNTS

INTRODUCTION

For many spectroscopic instruments such as spectrographs, monochromators, spectrophotometers, and similar instruments employing concave optical reflecting diffraction gratings, a major inherent optical disadvantage is that the diffracted image size (exit slit) is distorted and many times larger than the objective size (entrance slit). This phenomenon is basically due to astigmatism caused by, in large part, the conventional concave diffraction grating used in the instrument. In order to detect all the energy in such large diffracted images, very large area detectors must be used. These detectors, if available, would be very large in size and would be unacceptable for use especially in flight spectroscopic instruments. At the present time, small area detectors are used with much of the energy being lost. A solution to this problem is to use the aberration corrected holographic gratings that correct for astigmatism.

The purpose of this report is to present the design of holographic gratings that will in many cases solve the problem of astigmatism and in other cases the problem of coma which causes a loss in resolving power in spectroscopic instruments.

The first section of this report presents the theory and basic equations for designing holographic diffraction gratings. The remaining sections are devoted to the development of a computer program that calculates the necessary geometrical data which is one of many requirements that makes the fabrication of holographic gratings a reality. The computer program has been developed such that optimum recording parameters as a function of instrument parameters are determined that make astigmatism or coma zero at specified wavelengths for spectrographs based on the Rowland circle mount. When optimum recording parameters have been determined, the program will display, for the purpose of comparison, numerical tables of the performance for the holographic grating and equivalent conventional grating as a function of wavelength. This numerical comparison makes it possible to analyze the data and decide whether or not the holographic grating performance is better than the equivalent conventional grating relative to optical aberrations.

THEORY AND BASIC EQUATIONS FOR DESIGNING HOLOGRAPHIC SPHERICAL CONCAVE GRATINGS

Figure 1 shows the optical system for using and recording holographic gratings. The rectangular coordinate system is defined as follows: I is the origin at the vertex of the grating blank and the x-axis is normal to I. The x-y plane is defined by I and the two recording point sources C and D. Points A, M, and B are respectively, a self luminous point on the entrance slit, a point on the grating surface, and a point on the focused diffracted image from M at a wavelength λ in the n^{th} order. As a result of this geometry the aberrant optical path function for a conventional grating may be written as

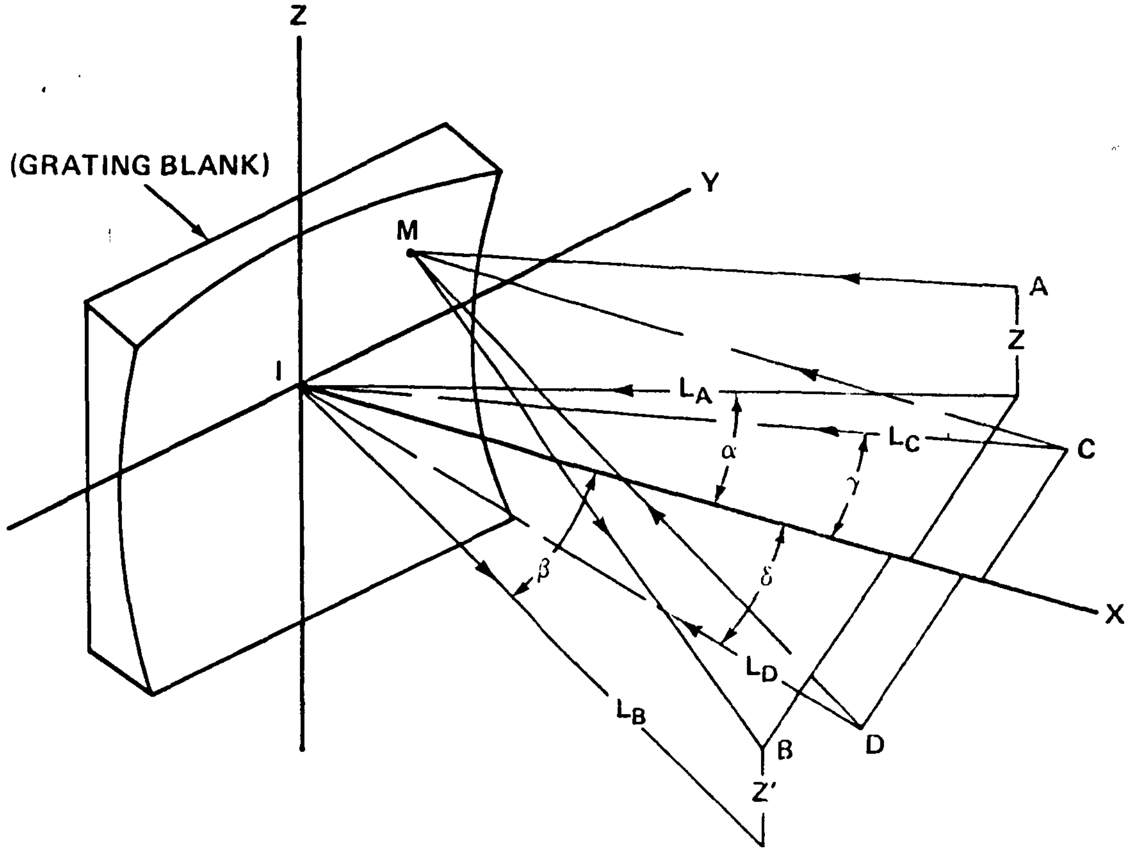


Figure 1. Schematic diagram of the optical system. A is a self luminous point on the entrance slit, M is a point on the n^{th} groove and B is the spectral image point. C and D are the recording point light source positions. The performance and recording parameters are defined as follows:

Performance Parameters:

- L_A is the distance from A (entrance slit) to the center of I of the grating.
- L_B is the distance from the diffracted image B to the center I of the grating.
- α is the angle of incidence.
- β is the diffraction angle.
- z is the object height.
- z' is the image height.

Recording Parameters:

- L_C is the distance from the point source C to the center I of the grating.
- L_D is the distance from the point source D to the center I of the grating.
- γ is the position angle for point source C relative to the normal to the grating.
- δ is the position angle for point source D relative to the normal to the grating.

$$\Delta M = AM + MB - (IA + IB) - KN\lambda \tag{1}$$

where K is the order of diffraction, λ is the diffracted image wavelength and N is the grating groove frequency.

When a grating blank coated with the photoresist is illuminated with coherent spherical waves originating from points C and D, grooves are recorded, after developing, in the photoresist in response to the interference fringes produced at the site of the grating blank. The interference fringes are formed according to the equation

$$N = \frac{MC - MD - (IC - ID)}{\lambda_o} \tag{2}$$

where λ_o is the recording laser wavelength.

Substituting eq. (2) into eq. (1) gives the aberrant optical path function

$$\Delta M = MA + MB - (IA + IB) - \frac{K\lambda}{\lambda_o} \left\{(MC - MD) - (IC - ID)\right\} \tag{3}$$

for the holographic grating.

The quantities on the right side of ΔM in eq. (3) are derived based on the coordinate system described in Figure 1 and the equations of a sphere. Since the results of these derivations are lengthy, we suggest that the reader see reference 1 for more detailed analysis. Therefore, it sufficies to say that after a series expansion is performed, the following aberrant optical path function ΔM is obtained.

$$\begin{aligned}\Delta M = & -Y\left[\sin\alpha + \sin\beta - \frac{K\lambda}{\lambda_o}\left\{\sin\gamma - \sin\delta\right\}\right] + \frac{Y^2}{2}[A_1] \\ & + \frac{Z^2}{2}[A_2] + \frac{Y^3}{2}[C_1] + \frac{YZ^2}{2}[C_2] + Y^4[S_1] \\ & + Y^2Z^2[S_2] + Z^4[S_3] + \ldots\end{aligned} \tag{4}$$

where Y is the width and Z is the height of the grating and

$$A_1 = \frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R} - \frac{K\lambda}{\lambda_o}\left\{\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R} - \left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\right\}$$

$$A_2 = \frac{1}{L_A} - \frac{\cos\alpha}{R} + \frac{1}{L_B} - \frac{\cos\beta}{R} - \frac{K\lambda}{\lambda_o}\left\{\frac{1}{L_C} - \frac{\cos\gamma}{R} - \left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)\right\} \tag{5}$$

$$C_1 = \frac{\sin\alpha}{L_A}\left(\frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R}\right) + \frac{\sin\beta}{L_B}\left(\frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R}\right)$$

$$- \frac{K\lambda}{\lambda_o}\left\{\frac{\sin\gamma}{L_C}\left(\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R}\right) - \left(\frac{\sin\delta}{L_D}\left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\right)\right\}$$

$$C_2 = \frac{\sin\alpha}{L_A}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) + \frac{\sin\beta}{L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)$$

$$- \frac{K\lambda}{\lambda_o}\left\{\frac{\sin\gamma}{L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{\sin\delta}{L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)\right\}$$

$$S_1 = \frac{1}{8R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{8L_A}\left(\frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R}\right)\left(\frac{1}{L_A} - \frac{\cos\alpha}{R} - \frac{5\sin^2\alpha}{L_A}\right)$$

$$+ \frac{1}{8R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) - \frac{1}{8L_B}\left(\frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R}\right)\left(\frac{1}{L_B} - \frac{\cos\beta}{R} - \frac{5\sin^2\beta}{L_B}\right)$$

$$- \frac{K\lambda}{\lambda_o}\left\{\frac{1}{8R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{8L_C}\left(\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R}\right)\left(\frac{1}{L_C} - \frac{\cos\gamma}{R} - \frac{5\sin^2\gamma}{L_C}\right)\right.$$

$$\left. - \left(\left(\frac{1}{8R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{8L_D}\left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\left(\frac{1}{L_D} - \frac{\cos\delta}{R} = \frac{5\sin^2\delta}{L_D}\right)\right)\right)\right\} \tag{5}$$

$$S_2 = \left(\frac{1}{4R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{4L_A}\left(\frac{1}{L_A} - \frac{\cos\beta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\alpha}{L_A{}^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right)\right.$$

$$\left. + \frac{1}{4R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) - \frac{1}{4L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\beta}{L_B{}^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)\right)$$

$$- \frac{K\lambda}{\lambda_o}\left\{\frac{1}{4R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{4L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\gamma}{L_C{}^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right)\right.$$

$$\left. - \left(\frac{1}{4R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{4L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\delta}{L_D{}^2}\left(\frac{1}{L_C} - \frac{\cos\delta}{R}\right)\right)\right\}$$

$$S_3 = \left(\frac{1}{8R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{8L_A}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right)^2 + \frac{1}{8R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)\right.$$

$$\left. - \frac{1}{8L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)^2\right) - \frac{K\lambda}{\lambda_o}\left\{\frac{1}{8R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{8L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right)^2\right.$$

$$\left. - \left(\frac{1}{8R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{8L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)^2\right)\right\}$$

Note that in the expressions of equation (5), L_A, L_B, α and β are the terms for the conventionally ruled grating, and L_C, L_D, γ, and δ are the terms related to the holographic contribution. R is the radius of curvature of the grating, K is the order of the diffracted wavelength, and λ_o is the recording wavelength. The aberration terms are defined as follows; A_1 is the horizontal diffracted image focus, A_2 is the astigmatism or vertical focusing term, C_1 and C_2 are coma terms and S_1, S_2, and S_3 are spherical aberration terms.

The conventional grating equation is given by

$$\sigma\,(\sin\alpha + \sin\beta) = K\lambda \tag{6}$$

and for the holographic grating σ is the effective grating constant and is defined by equation

$$\sigma = \frac{\lambda_o}{\sin\gamma - \sin\delta} \quad \text{where } \gamma > \delta \tag{7}$$

The preceding information describes the basic general theory for holographic gratings. What follows is an application of the general theory for a specific spectroscopic instrument; correcting astigmatism or coma at a specified wavelength for a Rowland circle spectrographic mount.

HOLOGRAPHIC GRATING DESIGN FOR THE ROWLAND CIRCLE SPECTROGRAPH

In order to design a holographic concave grating that has the Rowland circle as its focal curve; it is necessary to make the horizontal focusing term A_1 and the coma term C_1 zero at all wavelengths in equation (5). This condition is satisfied by

$$L_A = R\cos\alpha,\ L_B = R\cos\beta,\ L_C = R\cos\gamma \text{ and } L_D = R\cos\delta \tag{8}$$

The aberrant optical path function for condition (8) will now have the form

$$\Delta M = -Y\left[\sin\alpha + \sin\beta - \frac{K\lambda}{\lambda_o}\left\{\sin\gamma - \sin\delta\right\}\right] + \frac{Z^2}{2R}[A_2'] + \frac{YZ^2}{2R^2}[C_2'] + \frac{Y^4}{8R^3}[S_1'] + \frac{Y^2Z^2}{4R^3}[S_2'] + \frac{Z^4}{8R^3}[S_1{}^3] \tag{9}$$

and the expressions for astigmatism A_2' and coma C_2' in equation (5) reduce to

$$A_2' = \frac{\sin^2\alpha^*}{\cos\alpha^*} + \frac{\sin^2\beta^*}{\cos\beta^*} - \frac{K\lambda^*}{\lambda_o}\left\{\frac{\sin^2\gamma}{\cos\gamma} - \frac{\sin^2\delta}{\cos\delta}\right\} \tag{10}$$

and

$$C_2' = \frac{\sin^3 \alpha^*}{\cos^2 \alpha^*} + \frac{\sin^3 \beta^*}{\cos^2 \beta^*} - \frac{K\lambda^*}{\lambda_o}\left\{\frac{\sin^3 \gamma}{\cos^2 \gamma} - \frac{\sin^3 \delta}{\cos^2 \delta}\right\} \qquad (11)$$

where λ^* is the wavelength at which the aberrations are to be corrected to zero and β^* is calculated from

$$\sigma (\sin \alpha^* + \sin \beta^*) = K\lambda^* \qquad (12)$$

The recording parameters γ, δ, L_C, and L_D are determined for a chosen set of values σ, λ^*, and α^* to eliminate astigmatism A_2' or coma C_2' at a specified wavelength λ^*. If astigmatism A_2' is desired to be eliminated at λ^*, then the following set of equations must be solved;

$$\sigma (\sin \alpha^* + \sin \beta^*) = K\lambda^*, \qquad (12)$$

$$\sigma = \frac{\lambda_o}{\sin \gamma - \sin \delta} \qquad (7)$$

and equation (10), $A_2' = 0$. For this case, the recording angles γ and δ are chosen such that astigmatism A_2' is made zero at λ^*.

If one chooses to eliminate coma at a wavelength λ^*, then the following set of equations must be solved; (12), (7) and (11), $C_2' = 0$. For this case, the recording angles γ and δ are chosen such that C_2' is made zero at λ^*.

When the recording parameters γ and δ have been determined for a given set of σ, α^*, and λ^*, then the values of L_A, L_B, L_C and L_D are calculated from equation (8). The remaining aberrations S_1', S_2', and S_3' in equation (5) are calculated after the aberrations A_2' and C_2' have been made zero at λ^* for the values determined for γ and δ. The aberration calculations determined by the computer for astigmatism, coma, and spherical are independent of Y, Z, R, and the constants in the denominators of the expressions for the coefficients. In other words the values of the aberrations are pure numbers.

OVERALL LOGIC

In the first section, we presented the general theory of holographic concave gratings and applied the theory to designing concave holographic gratings, corrected for astigmatism or coma, for a spectrograph based on the Rowland circle mount.

In this section, we present the logical steps of the computer program that leads to the design of holographic gratings.

Step 1 requires that one selects the groove frequency, angle of incidence, correcting wavelength λ^*, and the radius of curvature R for the holographic grating.

Step 2; Based on the data of step 1, determine the angle of diffraction β^* at λ^*.

Step 3; The expression for astigmatism A_2' equation (10) is then scanned as a function of the recording angle γ to determine the optimum angles γ and δ that will make $A_2' = 0$ at λ^*. Successive values of γ are obtained by an equation of the form $\gamma = \gamma_i + \Delta\gamma$ where $\Delta\gamma$ is an incremental angle and chosen to equal 0.25°. Therefore the accuracy of γ is dependent on the value of $\Delta\gamma$; the smaller the incremental angle $\Delta\gamma$ the better the accuracy of γ.

Step 4; When the optimum recording angles γ and δ have been determined for correcting astigmatism A_2' at λ^*, then the performance of the grating relative to all aberrations as a function of wavelength over a chosen wavelength range is calculated for the holographic grating and displayed in the form of a table. For comparison, the performance of an equivalent conventional grating is also calculated and displayed for the same wavelength range.

The same logical process is employed for correcting coma C_2' (equation (11)), however, the optimum recording parameters are related to correcting coma.

A unique feature of the program is that it automatically calculates the optimum recording parameters for both astigmatism and coma corrections and then displays complete data for each aberration correction. This feature was included in the program so that the program user may select which aberration correction will best provide the optimum performance for all aberrations (astigmatism, coma, and spherical) throughout the desired wavelength range.

DESCRIPTION OF COMPUTER PROGRAM

The previous section gave the logical sequence for setting up the computer program. This section describes the computer program which consists of a main program and two subroutines.

The main program directs the flow of calculations and calls upon the subroutines to perform their various functions. The flow diagram (Figure 2) shows that the following events will be performed.

1. Input data cards are read.

2. Call CORECT. CORECT is a subroutine that determines the optimum recording parameter values for γ and δ such that astigmatism is corrected to zero at λ^*. This is achieved by simultaneous solution of equations (12), (7), and (10). Then this subroutine also automatically determines the optimum recording parameter values for γ

and δ to correct coma to zero at λ^*. This task is accomplished by simultaneous solution of equations (12), (7), and (11).

3. Call PRFORM. PRFORM is a subroutine that calculates the numerical values for all aberrations as a function of wavelength for both holographic and conventional gratings.

4. Output. This function displays the numerical values of the input data, recording parameters, and all aberrations for the holographic and conventional gratings as a function of wavelength in the form of a table.

MAIN PROGRAM FLOW DIAGRAM

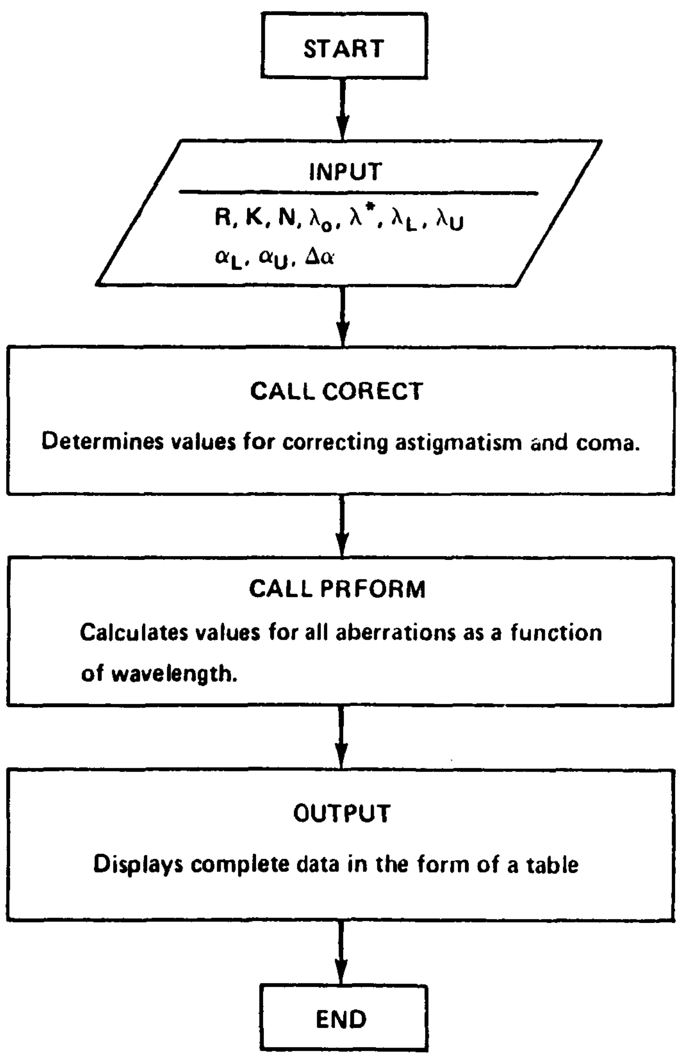


Figure 2. Main Program Flow Diagram.

INPUT DATA, DEFINITION OF TERMS AND DATA CARDS

This section describes the input data and defines the parameters that will be punched on the data cards so that successful operation of the program will be achieved.

DATA SET

The data set consist of 11 input parameters that must be properly presented on the data cards in order to make proper use of the program. The parameters are defined as follows:

1. R = radius of curvature in mm.

2. K = order of diffraction, where $K = \pm 1, \pm 2$, etc. The choice of negative or positive orders is at the discretion of the program user.

3. N = groove frequency in grooves/mm.

4. λ_o = laser recording wavelength in angstroms.

5. λ^* = correcting wavelength in angstroms.

6. λ_L = lower wavelength limit in angstroms for displaying the performance of the grating.

7. $\Delta\lambda$ = wavelength interval in angstroms for displaying the performance of the grating.

8. λ_U = upper wavelength limit in angstroms for displaying the performance of the grating.

9. α_L = lower angle of incidence in degrees decimal form.

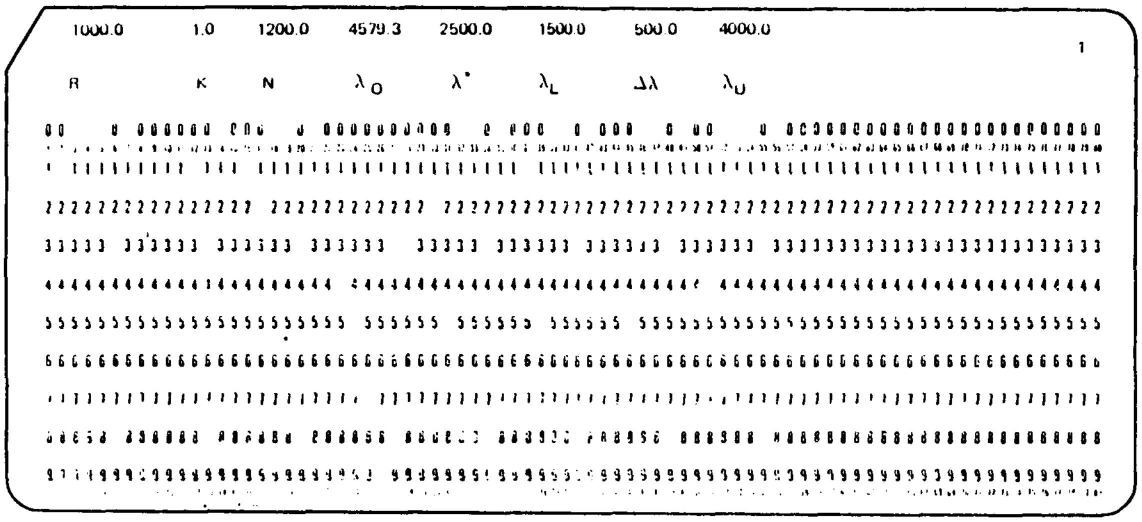
10. α_U = upper angle of incidence in degrees decimal form.

11. $\Delta\alpha$ = incremented angle of incidence in degrees decimal form.

α_L, α_U, and $\Delta\alpha$ require some explanation. The incremental angle of incidence $\Delta\alpha$ provides the program user the opportunity to obtain optimum recording parameters for successive angles of incidence at specified increments without punching data card sets for each desired angle of incidence. For example; if α_L and α_U are given respective input values 0.0° and 10.0° and $\Delta\alpha$ = 5.0°, then optimum recording parameters will be obtained for α = 0.0°, 5.0°, and 10.0°. Complete data will be displayed for each of the three angles of incidence. If the program user selects one input angle of incidence, then α_L and α_U have the same input value and $\Delta\alpha$ = 0.0°.

DATA CARDS

The order of the first eight input parameters must be punched in the order shown in the DATA SET section starting in column 1 in format F7.1 with seven columns reserved for each of the eleven parameters on the first data card and each parameter must include a decimal. The parameters α_L, α_U, and $\Delta\alpha$ are punched on the second data card in that order with seven columns reserved for each of these three parameters in F7.1 format and each parameter must include a decimal. Figure 3 shows a typical two card data set to illustrate the description stated above.



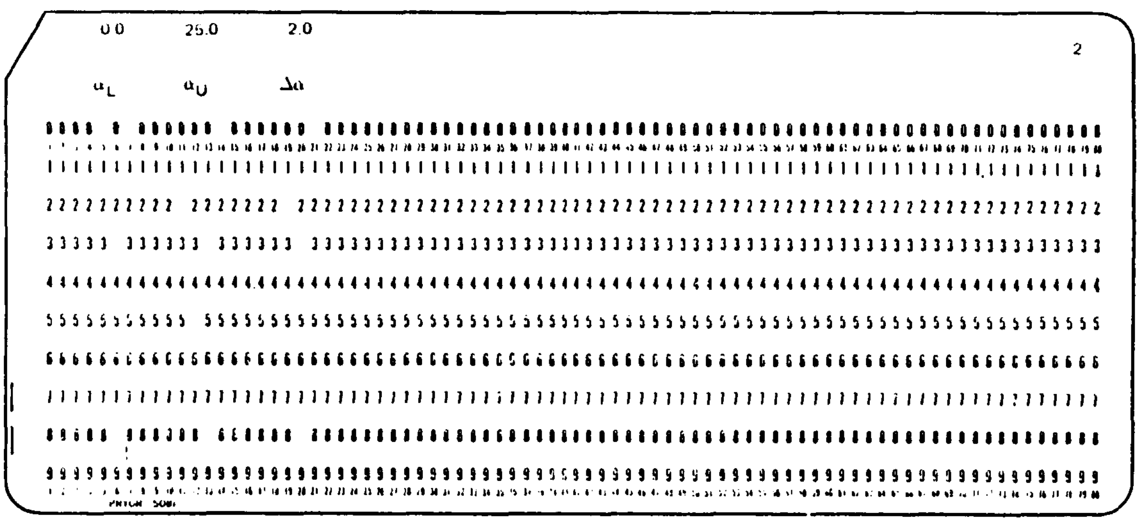


Figure 3.

NOTE:

1. The program user may include as many data sets as required in a single run of the program.
2. The values of all 11 input parameters must be punched on all data card sets.

PROGRAM EXAMPLE AND DATA DISPLAY

This section presents a typical example of the use of the program and also describes the output data in detail.

Example: Determine the optimum recording parameters γ and δ such that astigmatism or coma is made zero at 2500Å for angles of incidence $\alpha = 0.0°$ to $25.0°$ in the incremental angles of $2.0°$. The grating has 1200 L/mm with a radius of curvature of 1000 mm and will operate in the 1st order. The wavelength performance range is from 1500Å to 4000Å in 500Å intervals.

Solution: A data card set is punched using the data supplied in the example and punched in the order listed as follows:

First Card

1. $R = 1000.0$ mm
2. $K = +1.0$
3. $N = 1200$ grooves/mm
4. $\lambda_o = 4579.3$Å
5. $\lambda^* = 2500.0$Å
6. $\lambda_L = 1500.0$Å
7. $\Delta\lambda = 500.0$Å
8. $\lambda_U = 4000.0$Å

Second Card

9. $\alpha_L = 0.0°$
10. $\alpha_U = 25.0°$
11. $\Delta\alpha = 2.0°$

The output data for the example cited is shown in Figure 4. Output data for only one of the angles of incidence will be presented for the purpose of illustration.

A detailed description of the output data for correcting astigmatism or coma at 2500Å is as follows:

```
1  INPUT DATA...
2  CA=RCOS(ALFA);CB=RCOS(BETA);CC=RCOS(GAMA);CD=RCOS(DELTA)
3     R= 1000.00 MMRLAM= 4579.30ANG   K=     1.00      N= 1200.00 LINES PER MM
4  ***** OPTION= 1***ASTIGMATISM (A2) CORRECTED
5          TOTAL NUMBER OF ROOTS FOR THIS CASE= 1

6  ************ROOT NUMBER= 1*********************
   ***** OPTION= 1***ASTIGMATISM (A2) CORRECTED
7  LAMDA= 2500.00 ANG   ALFA= 0.180D 02 DEG BETA=-0.517D 00 DEG GAMA= 0.252D 02 DEG DELTA=-0.715D 01 DEG

8  HOLO..     A1= C.C      A2=-0.148D-07   C1= 0.0      C2=-0.196D-01   S1=-0.148D-07   S2=-0.266D-01   S3= 0.133D-01
9  CONV..     A1= 0.0      A2= 0.100D 00   C1= 0.0      C2= 0.326D-01   S1= 0.100D 00   S2= 0.122D 00   S3= C.899D-01

10 HOLOGRAPHIC GRATING...

11  LAMDA      BETA      A1       A2            C1       C2            S1           S2           S3
   (ANGS)     (DEG)

12  4000.0     5.84   C.0     -0.307D-01    0.0     -0.459D-01   -0.307D-01   -0.842D-01   -0.354D-02
    3500.0     6.37   0.0     -0.279D-01    0.0     -0.392D-01   -0.279D-01   -0.733D-01   -0.516D-02
    3000.0     2.92   0.C     -0.176D-01    0.0     -0.300D-01   -0.176D-01   -0.537D-01    0.510D-03
    2500.0    -0.52   C.0     -0.148D-07    0.0     -0.196D-01   -0.148D-07   -0.266D-01    0.133D-01
    2000.0    -3.96   C.C      0.248D-01    0.0     -0.952D-02    0.248D-01    0.778D-02    0.353D-01
    1500.0    -7.41   0.0      0.569D-01    0.0     -0.917D-03    0.569D-01    0.500D-01    0.604D-01
13 CONVENTIONAL GRATING...

14  LAMDA      BETA      A1       A2            C1       C2            S1           S2           S3
   (ANGS)     (DEG)
15  4000.0     5.84   C.0      0.130D 00    0.0      0.378D-01    0.130D 00    0.153D 00    0.119D C0
    3500.0     6.37   0.C      0.113D 00    0.0      0.340D-01    0.113D 00    0.134D 00    0.102D 00
    3000.0     2.92   0.0      0.103D 00    0.0      0.328D-01    0.103D 00    0.124D 00    0.924D-01
    2500.0    -0.52   C.C      0.100D 00    0.0      0.326D-01    0.100D 00    0.122D 00    0.899D-01
    2000.0    -3.96   C.C      0.105D 00    0.0      0.322D-01    0.105D 00    0.126D 00    0.946D-01
    1500.0    -7.41   0.0      0.117D 00    0.0      0.304D-01    0.117D 00    0.139D 00    0.106D 00

16 ***** OPTION= 2***********COMA (C2) CORRECTED
17         TOTAL NUMBER OF ROOTS FOR THIS CASE= 2
```

Figure 4.

18 **************ROOT NUMBER= 1**********************
***** OPTION= 2**********COMA (C2) CORRECTED

19 LAMDA= 2500.00 ANG ALFA= 0.180D 02 DEG BETA=-0.517D 00 DEG GAMA= 0.111D 02 DEG DELTA=-0.210D 02 DEG

20	HOLO..	A1= 0.0	A2= 0.155D 00	C1= 0.0	C2=-0.127D-07	S1= 0.155D 00	S2= 0.196D 00	S3= 0.134D 00
21	CONV..	A1= 0.0	A2= 0.100D 00	C1= 0.0	C2= 0.326D-01	S1= 0.100D 00	S2= 0.122D 00	S3= 0.899D-01

22 HOLOGRAPHIC GRATING...

23	LAMDA (ANGS)	BETA (DEG)	A1	A2	C1	C2	S1	S2	S3
24	4000.0	9.84	0.0	0.217D 00	0.0	-0.144D-01	0.217D 00	0.272D 00	0.189D 00
	3500.0	6.37	0.0	0.189D 00	0.0	-0.117D-01	0.189D 00	0.239D 00	0.164D 00
	3000.0	2.92	0.0	0.168D 00	0.0	-0.639D-02	0.169D 00	0.214D 00	0.145D 00
	2500.0	-0.52	0.0	0.155D 00	0.0	-0.127D-07	0.155D 00	0.196D 00	0.134D 00
	2000.0	-3.96	0.0	0.146D 00	0.0	0.620D-02	0.149D 00	0.180D 00	0.130D 00
	1500.0	-7.41	0.0	0.150D 00	0.0	0.105D-01	0.150D 00	0.184D 00	0.133D 00

25 CONVENTIONAL GRATING...

26	LAMDA (ANGS)	BETA (DEG)	A1	A2	C1	C2	S1	S2	S3
27	4000.0	9.84	0.0	0.130D 00	0.0	0.378D-01	0.130D 00	0.153D 00	0.119D 00
	3500.0	6.37	0.0	0.113D 00	0.0	0.340D-01	0.113D 00	0.134D 00	0.102D 00
	3000.0	2.92	0.0	0.103D 00	0.0	0.328D-01	0.103D 00	0.124D 00	0.924D-01
	2500.0	-0.52	0.0	0.100D 00	0.0	0.326D-01	0.100D 00	0.122D 00	0.899D-01
	2000.0	-3.96	0.0	0.105D 00	0.0	0.323D-01	0.105D 00	0.126D 00	0.946D-01
	1500.0	-7.41	0.0	0.117D 00	0.0	0.304D-01	0.117D 00	0.139D 00	0.106D 00

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Figure 4. (Continued)

Line 1 is self explanatory and refers to the next two lines.

Line 2 shows the equations for calculating L_A, L_B, L_C and L_D.

Line 3 shows the radius of curvature R, recording wavelength λ_0 = RLAM, grating order K, and the groove frequency N.

Line 4 shows that astigmatism is being corrected and is indicated by option = 1. Option = 1 is an internal part of the program and is not an input parameter.

Line 5 shows the number of solutions available at the correcting wavelength λ^*.

Line 6 indicates that the following data refers to the first solution.

Line 7 shows the values of the correcting wavelength λ^* = LAMDA, angle of incidence α = ALFA, diffracted image angle β = BETA, recording angle γ = GAMA and recording angle δ = DELTA.

Line 8 shows the values of the aberrations corrected at λ^*. Note the value for astigmatism A_2 is essentially zero.

Line 9 shows the values of the aberrations for the conventional equivalent grating at λ^*. Notice how much greater the value of astigmatism is at λ^* compared to the value for the holographic grating in Line 8.

Line 10 indicates that the data in Lines 11 and 12 refer to the holographic grating.

Line 11 shows the titles for the performance of the holographic grating. LAMDA is the wavelength at which the grating is evaluated relative to the aberrations. BETA is the diffraction angle. The aberration titles A_1, A_2, C_1, C_2, S_1, S_2 and S_3 have been defined in the text.

Line 12 shows the values of the wavelength, diffraction angle, and aberrations for the performance of the grating. Note the values of the aberrations at 2500Å and compare with Line 8.

Line 13 indicates that the table that follows refers to the performance of an equivalent conventional grating.

Lines 14 and 15 refer to the conventional grating. Compare the values of this table with the values in the holographic grating performance table. Note the reduction in the aberration values for the holographic grating.

Lines 16 indicates that the following data is for correcting coma and is indicated by option = 2. Option = 2 is inherent to the program and is not an input parameter.

Line 17 indicates that for the angle of incidence shown in Line 19, there are two solutions for correcting coma.

Line 18 shows that the first solution will be evaluated for coma. The output data for the second solution is not shown.

Lines 19 through 27 are defined in the same way as Lines 6 through 15 except that they refer to coma.

REFERENCES

Pieuchard, G. and J. Flamand, Goddard Space Flight Center Report, Contract No. NASW 2146, March, 1972.

SIMULTANEOUS CORRECTION OF ASTIGMATISM, COMA, AND FIRST SPHERICAL ABERRATION TERM OF HOLOGRAPHIC CONCAVE GRATINGS FOR ROWLAND CIRCLE SPECTROGRAPHS

SIMULTANEOUS CORRECTION OF ASTIGMATISM, COMA, AND FIRST SPHERICAL ABERRATION TERM OF HOLOGRAPHIC CONCAVE GRATINGS FOR A ROWLAND CIRCLE SPECTROGRAPH

INTRODUCTION

When designing spectroscopic instruments such as spectrographs, monochromators, spectrophotometers and other instruments employing concave optical reflecting diffraction gratings, one of the most important optical design criteria is to design the optical system such that optical aberrations are reduced or eliminated over the desired wavelength range of operation. The most notorious aberration is normally astigmatism because the diffracted images are magnified in the vertical direction. As a result, large area detectors are required to sense all the energy in the diffracted image or, as is the usual case, available small area detectors are used at the expense of losing a great deal of energy in the diffracted image.

However, with the advent of aberration corrected concave holographic optical reflecting gratings, astigmatism and other aberrations have been reduced or eliminated at specified wavelengths. Recent publications have shown that for certain spectroscopic instrument designs incorporating corrective type holographic gratings either astigmatism or coma may be minimized over a desired wavelength range or astigmatism or coma may be eliminated at specified wavelengths.(1,2,3,4) However, the aberrations can not be corrected simultaneously at specified wavelengths. The purpose of this paper is to present the theory and basic equations that lead to the design of concave holographic diffraction gratings for Rowland circle spectrographs that do eliminate astigmatism, coma, and the first spherical aberration term simultaneously at specified wavelengths. However, the simultaneous elimination or correction to zero of these aberrations occurs at wavelengths that are greater than or equal to the laser recording wavelength.

A computer program was also developed to numerically analyze the theory, determine the optimum instrument performance and recording parameters necessary for grating fabrication. The program also displays the performance, for comparison, of both the holographic grating and equivalent conventional grating as a function of wavelength.

THEORY AND BASIC EQUATIONS FOR DESIGNING HOLOGRAPHIC SPHERICAL CONCAVE GRATINGS

Figure 1 shows the optical system for using and recording a concave spherical holographic grating. The rectangular coordinate system is defined as follows: I is the origin at the vertex of the grating blank and the x-axis is normal to I. The x-y plane is defined by I and the two recording point sources C and D. Points A, M, and B are, respectively, a self luminous point on the entrance slit, a point on the grating surface, and a point on the diffracted image from M at a wavelength λ in the n^{th} order. A knowledge of the

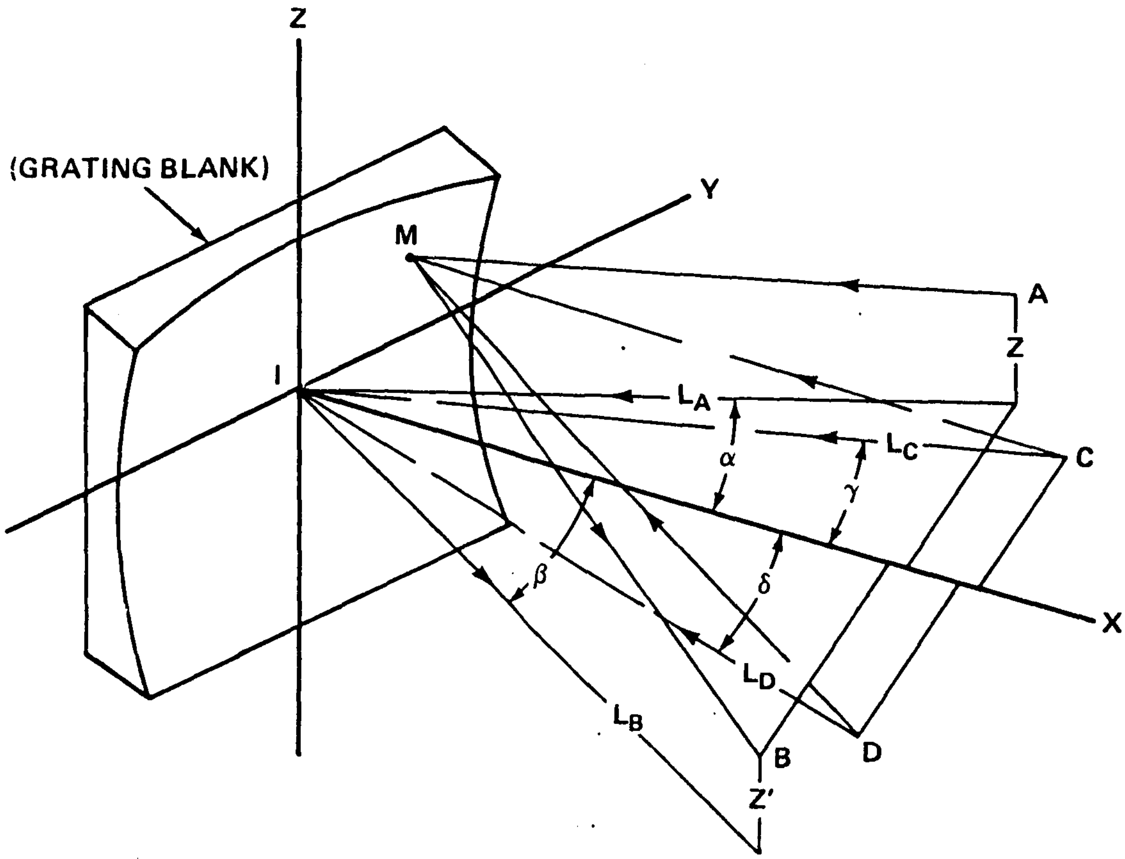


Figure 1. Schematic diagram of the optical system. A is a self luminous point on the entrance slit, M is a point on the n^{th} groove and B is the spectral image point. C and D are the recording point light source positions. The performance and recording parameters are defined as follows:

Performance Parameters:

- L_A is the distance from A (entrance slit) to the center of I of the grating.
- L_B is the distance from the diffracted image B to the center I of the grating.
- α is the angle of incidence.
- β is the diffraction angle.
- z is the object height.
- z′ is the image height.

Recording Parameters:

- L_C is the distance from the point source C to the center I of the grating.
- L_D is the distance from the point source D to the center I of the grating.
- γ is the position angle for point source C relative to the normal to the grating.
- δ is the position angle for point source D relative to the normal to the grating.

geometry of the optical system, Figure 1, leads to writing the aberrant optical path function ΔM for the conventional grating as

$$\Delta M = AM + MB - (IA + IB) - KN\lambda \tag{1}$$

where K is the order of diffraction, λ is the diffracted wavelength and N is the grating groove frequency.

When a grating blank coated with a photoresist is illuminated by coherent spherical wave fronts originating from points C and D, grooves are recorded, after development, in the photoresist in response to the interference fringes produced at the site of the grating blank. The interference fringes are formed according to the equation

$$N = \frac{MC - MD - (IC - ID)}{\lambda_o} \tag{2}$$

where λ_o is the recording laser wavelength.

Substituting eq. (2) into eq. (1) gives the aberrant optical path function

$$\Delta M = MA + MB - (IA + IB) - \frac{K\lambda}{\lambda_o}\left\{(MC - MD) - (IC - ID)\right\} \tag{3}$$

for the holographic grating.

The quantities on the right side of ΔM in equation (3) are derived based on the coordinate system described in Figure 1 and the equation of a sphere. Since these derivations are lengthy, we suggest the reader see reference 4 for a more detailed analysis. Therefore it suffices to say that after a series expansion is performed, the following result for ΔM is obtained.

$$\Delta M = -Y\left[\sin\alpha + \sin\beta - \frac{K\lambda}{\lambda_o}\left\{\sin\gamma - \sin\delta\right\}\right] + \frac{Y^2}{2}[A_1] \tag{4}$$

$$+\frac{Z^2}{2}[A_2] + \frac{Y^3}{2}[C_1] + \frac{YZ^2}{2}[C_2] + Y^4[S_1]$$

$$+ Y^2Z^2[S_2] + Z^4[S_3] + \ldots$$

where Y is the width and Z is the height of the grating and

$$A_1 = \frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R} + \frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R} - \frac{K\lambda}{\lambda_o}\left\{\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R} - \left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\right\}$$

$$A_2 = \frac{1}{L_A} - \frac{\cos\alpha}{R} + \frac{1}{L_B} - \frac{\cos\beta}{R} - \frac{K\lambda}{\lambda_o}\left\{\frac{1}{L_C} - \frac{\cos\gamma}{R} - \left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)\right\} \tag{5}$$

$$
\begin{aligned}
C_1 = {} & \frac{\sin\alpha}{L_A}\left(\frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R}\right) + \frac{\sin\beta}{L_B}\left(\frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R}\right) \\
& - \frac{K\lambda}{\lambda_o}\left\{\frac{\sin\gamma}{L_C}\left(\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R}\right) - \left(\frac{\sin\delta}{L_D}\left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\right)\right\} \\
C_2 = {} & \frac{\sin\alpha}{L_A}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) + \frac{\sin\beta}{L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) \\
& - \frac{K\lambda}{\lambda_o}\left\{\frac{\sin\gamma}{L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{\sin\delta}{L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)\right\} \\
S_1 = {} & \frac{1}{8R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{8L_A}\left(\frac{\cos^2\alpha}{L_A} - \frac{\cos\alpha}{R}\right)\left(\frac{1}{L_A} - \frac{\cos\alpha}{R} - \frac{5\sin^2\alpha}{L_A}\right) \\
& + \frac{1}{8R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) - \frac{1}{8L_B}\left(\frac{\cos^2\beta}{L_B} - \frac{\cos\beta}{R}\right)\left(\frac{1}{L_B} - \frac{\cos\beta}{R} - \frac{5\sin^2\beta}{L_B}\right) \\
& - \frac{K\lambda}{\lambda_o}\Bigg\{\frac{1}{8R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{8L_C}\left(\frac{\cos^2\gamma}{L_C} - \frac{\cos\gamma}{R}\right)\left(\frac{1}{L_C} - \frac{\cos\gamma}{R} - \frac{5\sin^2\gamma}{L_C}\right) \\
& - \Bigg(\Bigg(\frac{1}{8R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{8L_D}\left(\frac{\cos^2\delta}{L_D} - \frac{\cos\delta}{R}\right)\left(\frac{1}{L_D} - \frac{\cos\delta}{R} = \frac{5\sin^2\delta}{L_D}\right)\Bigg)\Bigg)\Bigg\} \qquad (5) \\
S_2 = {} & \Bigg(\frac{1}{4R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{4L_A}\left(\frac{1}{L_A} - \frac{\cos\beta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\alpha}{L_A{}^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) \\
& + \frac{1}{4R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) - \frac{1}{4L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\beta}{L_B{}^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) \\
& - \frac{K\lambda}{\lambda_o}\Bigg\{\frac{1}{4R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{4L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\gamma}{L_C{}^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) \\
& - \Bigg(\frac{1}{4R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{4L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)^2 + \frac{3}{4}\frac{\sin^2\delta}{L_D{}^2}\left(\frac{1}{L_C} - \frac{\cos\delta}{R}\right)\Bigg)\Bigg\} \\
S_3 = {} & \Bigg(\frac{1}{8R^2}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right) - \frac{1}{8L_A}\left(\frac{1}{L_A} - \frac{\cos\alpha}{R}\right)^2 + \frac{1}{8R^2}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right) \\
& - \frac{1}{8L_B}\left(\frac{1}{L_B} - \frac{\cos\beta}{R}\right)^2\Bigg) - \frac{K\lambda}{\lambda_o}\Bigg\{\frac{1}{8R^2}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right) - \frac{1}{8L_C}\left(\frac{1}{L_C} - \frac{\cos\gamma}{R}\right)^2 \\
& - \Bigg(\frac{1}{8R^2}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right) - \frac{1}{8L_D}\left(\frac{1}{L_D} - \frac{\cos\delta}{R}\right)^2\Bigg)\Bigg\}
\end{aligned}
$$

Note, that in the expressions for equation (5), L_A, L_B, α, and β are the terms for the conventionally ruled grating and L_C, L_D, γ, and δ are the terms related to the holographic contribution. R is the radius of curvature of the grating and K is the order. λ_o is the recording laser wavelength. The expressions in equation (5) are defined as follows: A_1 is the horizontal focusing term, A_2 is the astigmatism or vertical focusing term, C_1 and C_2 are coma terms and S_1, S_2, S_3 are spherical aberration terms.

The grating equation is given by

$$\sigma\ (\sin\alpha + \sin\beta) = K\lambda \tag{6}$$

and for the holographic grating, σ is the effective grating constant defined by

$$\sigma = \frac{\lambda_o}{\sin\gamma - \sin\delta} \quad \text{where } \gamma > \delta \tag{7}$$

The above description presents the general theory and basic equations for designing aberration corrected holographic gratings. We will now apply the theory to design a holographic grating that simultaneously corrects astigmatism, coma, and the first spherical aberration term at a specified wavelength.

HOLOGRAPHIC GRATING DESIGN FOR ROWLAND CIRCLE SPECTROGRAPH

A_1 and C_1 in equation (5) must be made zero in order to design a holographic grating that has the Rowland circle as its focal curve. The solution for this condition is:

$$L_A = R\cos\alpha,\ L_B = R\cos\beta,\ L_C = R\cos\gamma \text{ and } L_D = R\cos\delta \tag{8}$$

Substitution of equation (8) into the aberrant optical path function reduces equation (4) to

$$\Delta M = -Y[\sin\alpha + \sin\beta - \frac{K\lambda}{\lambda_o}\left\{\sin\gamma - \sin\delta\right\}] + \frac{Z^2}{2R}[A_2']$$

$$+\frac{YZ^2}{2R^2}[C_2'] + \frac{Y^4}{8R^3}[S_1'] + \frac{Y^2Z^2}{4R^3}[S_2'] + \frac{Z^4}{8R^3}[S_3'] \tag{9}$$

where the expressions in equation (5) take the form

$$A_2' = \frac{\sin^2\alpha^*}{\cos\alpha^*} + \frac{\sin^2\beta^*}{\cos\beta^*} - \frac{K\lambda^*}{\lambda_o}\left\{\frac{\sin^2\gamma}{\cos\gamma} - \frac{\sin^2\delta}{\cos\delta}\right\} \tag{10}$$

$$C_2' = \frac{\sin^3 \alpha^*}{\cos^2 \alpha^*} + \frac{\sin^3 \beta^*}{\cos^2 \beta^*} - \frac{K\lambda^*}{\lambda_o} \left\{ \frac{\sin^3 \gamma}{\cos^2 \gamma} - \frac{\sin^3 \delta}{\cos^2 \delta} \right\}$$

$$S_1' = \frac{\sin^2 \alpha^*}{\cos \alpha^*} + \frac{\sin^2 \beta^*}{\cos \beta^*} - \frac{K\lambda^*}{\lambda_o} \left\{ \frac{\sin^2 \gamma}{\cos \gamma} - \frac{\sin^2 \delta}{\cos \delta} \right\}$$

$$S_2' = \frac{\sin^2 \alpha^* (1 + \sin^2 \alpha^*)}{\cos^3 \alpha^*} + \frac{\sin^2 \beta^* (1 + \sin^2 \beta^*)}{\cos^3 \beta^*} \tag{10}$$

$$- \frac{K\lambda^*}{\lambda_o} \left\{ \frac{\sin^2 \gamma (1 + \sin^2 \gamma)}{\cos^3 \gamma} - \frac{\sin^2 \delta (1 + \sin^2 \delta)}{\cos^3 \delta} \right\}$$

$$S_3' = \frac{\sin^2 \alpha}{\cos^3 \alpha} (2 \cos^2 \alpha^* - 1) + \frac{\sin^2 \beta^*}{\cos^3 \beta^*} (2 \cos^2 \beta^* - 1)$$

$$- \frac{K\lambda^*}{\lambda_o} \left\{ \frac{\sin^2 \gamma}{\cos^3 \gamma} (2 \cos^2 \gamma - 1) - \frac{\sin^2 \delta}{\cos^3 \delta} (2 \cos^2 \delta - 1) \right\}$$

λ^* is the wavelength at which the aberrations are corrected to zero and β^* is calculated from

$$\sigma (\sin \alpha^* + \sin \beta^*) = K\lambda^* \tag{11}$$

Note that the groove frequency of the grating is given by $N = \dfrac{1}{\sigma}$.

SIMULTANEOUS CORRECTION OF ASTIGMATISM, COMA, AND FIRST SPHERICAL ABERRATION TERM AT λ^*

The simultaneous elimination of astigmatism, coma, and first spherical aberration term at λ^* depends on the instrument and recording parameters. For given instrumental parameters σ and λ^* there are specific angles of incidence α^* for which the recording angles γ and δ are chosen such that astigmatism, coma, and first spherical aberration term are simultaneously made zero. These aberration corrections are accomplished by simultaneously solving the following set of equations:

$$\sigma (\sin \alpha^* + \sin \beta^*) = K\lambda^*, \tag{11}$$

$$\sigma = \frac{\lambda_o}{\sin \gamma - \sin \delta} \tag{7}$$

and $A_2' = C_2' = 0$ in equation (10). Since the expression for S_1' is identical to A_2', the first spherical aberration term S_1 is automatically zero. A numerical analysis of the above theory shows that solutions exist only for $\lambda^* \geqslant \lambda_0$. The numerical analysis also shows that there are one or more angles of incidence α^* for each correcting wavelength λ^*, depending upon groove frequency for which $A_2' = C_2' = S_1' = 0$. Figure 2 shows some of a family of curves which for a given groove frequency and correcting λ^*, the angles of incidence α^* and the recording angle δ may be obtained such that $A_2' = C_2' = S_1' = 0$. The groove frequency is shown for each curve and the correcting wavelengths are indicated at different points along that curve. For example, at a groove frequency of 1200 L/mm and a correcting wavelength at 5000 Å, there are three angles of incidence (5.07°, 30.77° and 43.16°) and two corresponding recording angles δ(−2.83° and 7.01°) where the aberrations may be simultaneously corrected. It is interesting to note that as the grating groove frequency increases, the number of incident angles α^* and range of correcting wavelength decreases.

The diffracted angle β^* and other recording angle γ are calculated by equations (11) and (7) respectively. After the instrument and recording angles have been determined, the remaining instrument parameter values L_A, L_B, and recording parameter values L_C, L_D are calculated using expressions in equation (8) along with the value of the radius curvature R.

COMPUTER PROGRAM

In the first part of this paper, we have presented the theory and basic equations necessary to design holographic gratings that are aberration corrected at specified wavelengths at or above the laser recording wavelength for Rowland circle spectrographic mounts. We have also presented data (Figure 2) that shows the different angles of incidence that could be used to design an optical system based upon a specified groove frequency and correcting wavelength that eliminates astigmatism, coma, and first spherical aberration term simultaneously. Now we present the computer program that made it possible to numerically analyze the theory and calculate the optimum performance and grating fabrication parameters. The program also displays the performance of the holographic grating and equivalent conventional grating relative to all the aberrations as a function of wavelength.

DESCRIPTION OF COMPUTER PROGRAM

The computer program consists of a main program and four subroutines. The main program directs the flow of calculations and calls upon the subroutines to perform their various functions. The flow diagram (Figure 3) shows the events that will be performed.

The algorithm may be summarized as follows: Assume that the radius of curvature, groove frequency, and correcting wavelength has been selected, then an angle of incidence α_1 = 0.0° is chosen and the corresponding diffracted angle β is calculated. Based on the above

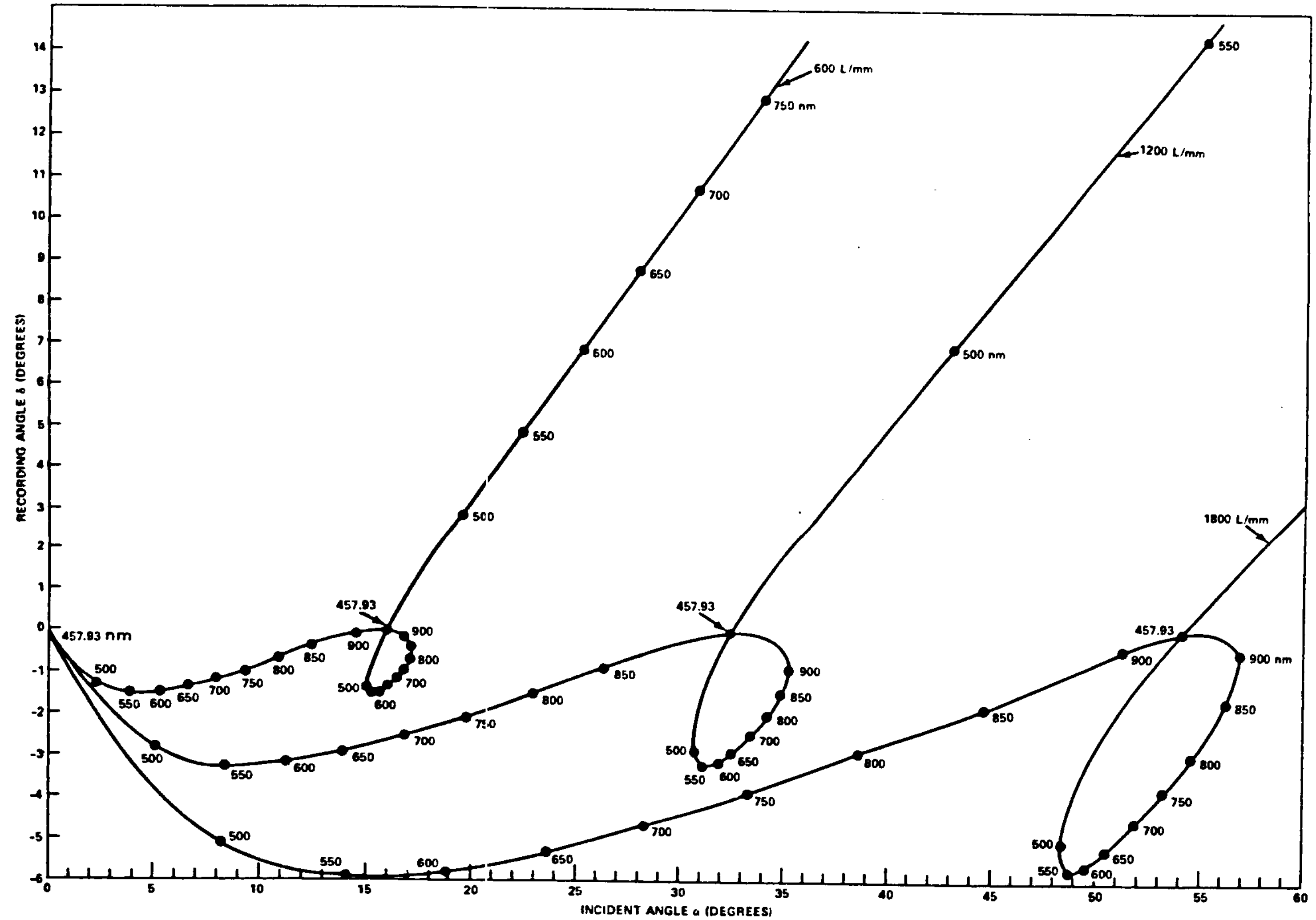


Figure 2. Family of curves showing the wavelengths in nanometers at which $A_2 = C_2 = S_1 = 0$. The correcting wavelength in nm is along each curve and is a function of the recording angle δ and the incident angle α. The groove frequency is shown at the end of each curve.

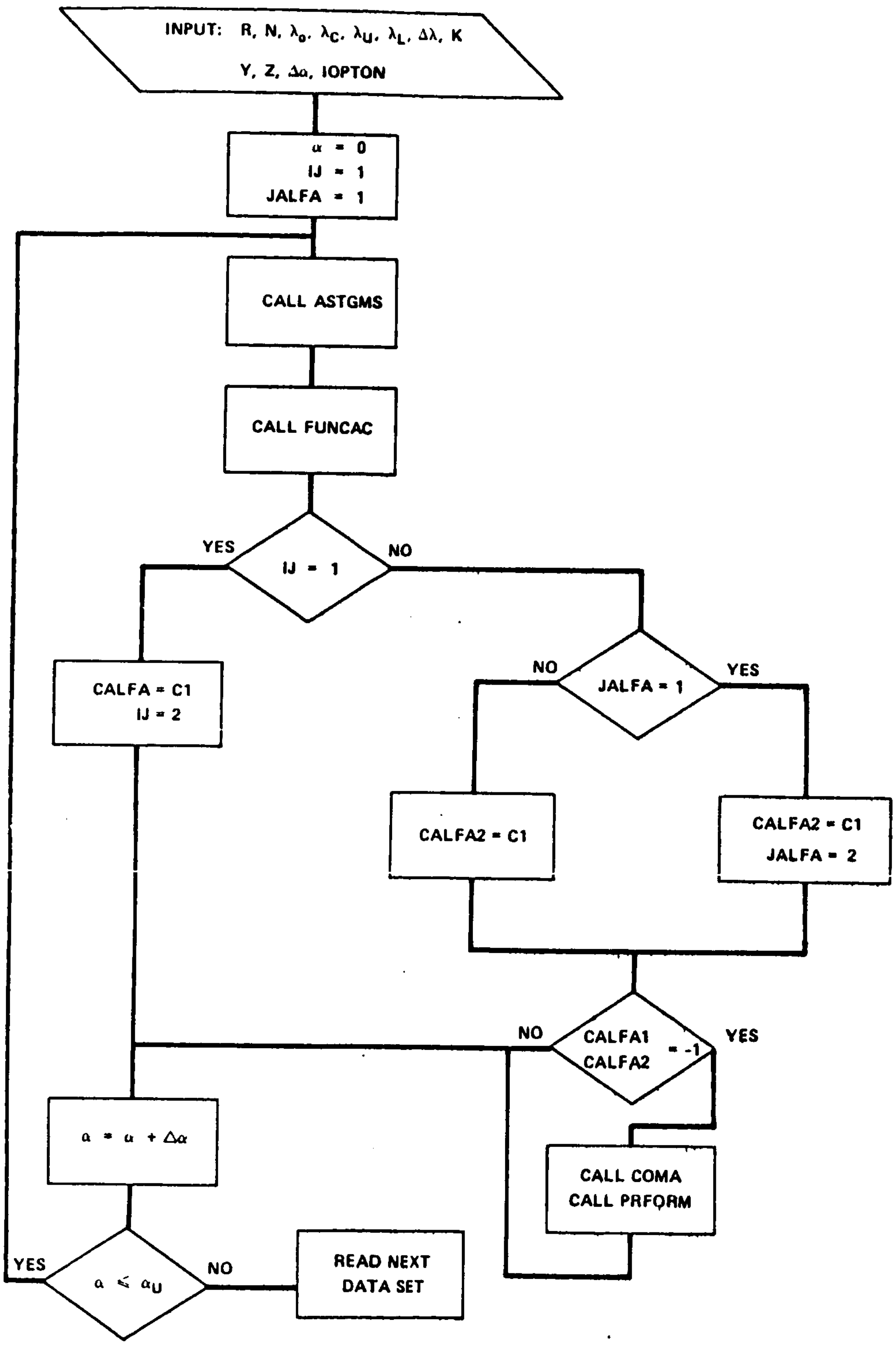


Figure 3. Program Flow Diagram.

parameters, the recording parameters γ_1 and δ_1 are determined such that $A_2 = 0$. The above procedure is repeated at another angle of incidence α_2, which is determined by an equation of the form $\alpha_2 = \alpha_1 + \Delta\alpha$; where α_1 is the previous angle of incidence and $\Delta\alpha$ is a very small incremental angle. At this point, there are two sets of parameters, α_1, β_1, γ_1, δ_1, and α_2, β_2, γ_2, δ_2 for which $A_2 = 0$. Note that A_2 can be made zero at any angle of incidence. For these two sets of parameters, two coma values for C_2 corresponding to $C_2(\alpha_1)$ and $C_2(\alpha_2)$ are calculated. If the values of the C_2 terms have opposite signs, then there exists a value α between α_1 and α_2 for which $A_2 = C_2 = 0$ for the same values of α, β, γ, and δ. The values of α and associated parameters are determined by a modification of Newton's method.

However, if $C_2(\alpha_1)$ and $C_2(\alpha_2)$ have the same sign then there isn't any value of α between α_1 and α_2 for which $A_2 = C_2 = 0$. When this happens, we set $\alpha_3 = \alpha_2 + \Delta\alpha$ and calculate the corresponding angles β_3, γ_3, and δ_3 such that $A_2(\alpha_3) = 0$. Then $C_2(\alpha_3)$ is calculated and the sign is compared with $C_2(\alpha_2)$. Again, if the signs are opposite there is another value of α between α_2 and α_3 such that $A_2 = C_2 = 0$. This process is repeated until all angles of incidence between 0° and 90° have been evaluated and only those angles of incidence are selected which satisfy the condition that for a certain α there is a β, γ, and δ that produces $A_2 = C_2 = 0$ for a specified groove frequency, radius of curvature and correcting wavelength. Since the equations for A_2 and S_1 are identical, then S_1 is also zero.

The algorithm is supported by four subroutines. Subroutine ASTGSM calculates the parameters required to make astigmatism zero at angles of incidence α.

Subroutine FUNCAC calculates the values of the coma terms based on the parameters used to make $A_2 = 0$. Then it compares the signs of the coma terms; if opposite this subroutine will determine the angle of incidence and related parameters that make coma zero. If the signs are the same, it returns the problem to subroutine ASTGSM and the process is repeated.

Subroutine Coma calculates the values of α, β, γ and δ such that $C_2 = 0$, when $A_2 = 0$ for the same set of parameters.

Subroutine PRFORM calculates and displays in the form of a table the numerical values of each aberration for the holographic grating and equivalent conventional grating as a function of wavelength.

INPUT DATA, DEFINITION OF TERMS AND DATA CARDS

This section describes the input data and defines the parameters that will be punched on the data cards so that successful operation of the program will be achieved.

(A) DATA SET

The data set consists of 12 parameters that must be properly presented on the data cards in order to successfully use the computer program. These parameters are defined as follows:

1. R = radius of curvature in mm.

2. N = groove frequency in grooves per mm.

3. λ_0 = laser recording wavelength in angstroms.

4. λ^* = correcting wavelength in angstroms.

5. λ_L = lower wavelength limit in angstroms for displaying the performance of the grating.

6. λ_U = upper wavelength limit in angstroms for displaying the performance of the grating.

7. $\Delta\lambda$ = wavelength interval in angstroms for displaying the performance of the grating.

8. K = order of diffraction, where K = ±1, ±2, etc. The choice of negative or positive orders is at the discretion of the program user.

9. Y = grating width in mm.

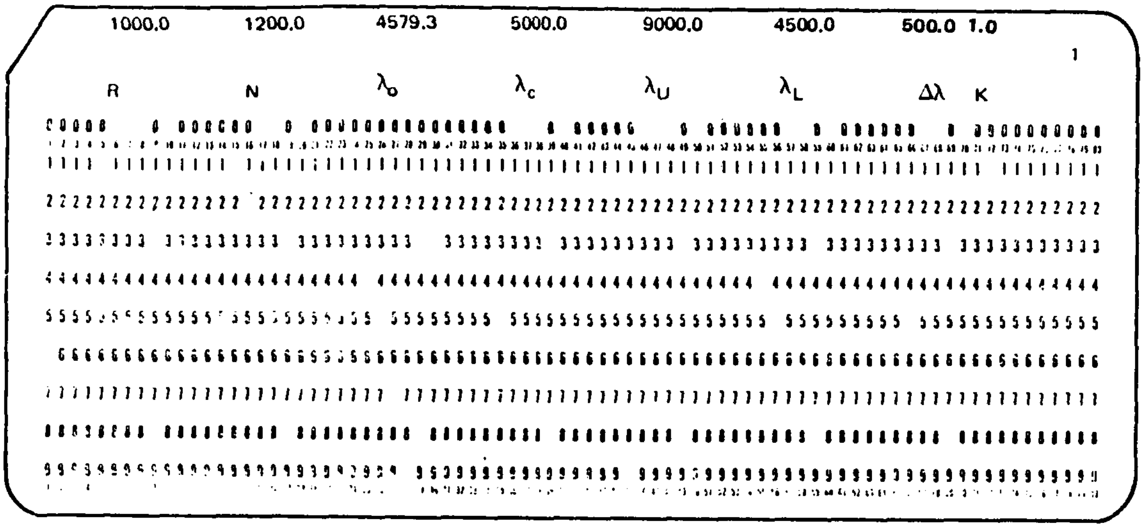
10. Z = grating height in mm.

11. $\Delta\alpha$ = incremental angle in degrees decimal form. The smaller the incremental angle, the more accurate the successive values of α.

12. IOPTION = Selects whether or not the coefficients Y and Z should be included in the aberration values. If IOPTION = 1 is selected, then the aberrations are calculated without the coefficients. If IOPTION = 2 is selected, then the aberrations calculated include the coefficients.

(B) DESCRIPTION OF DATA CARDS AND SAMPLE DATA CARDS

The order of the first eight input parameters must be punched in the order shown in (A) starting in column 1 in F10.1 format with 10 columns reserved for each of the seven parameters and each parameter must include a decimal. The eighth parameter K is in I2 format and punched in columns 71, 72. The next four parameters are punched on the second card where parameters Y, Z and $\Delta\alpha$ are format F10.1 and IOPTION is in I2 format. Figure 4 shows a typical two card data set to illustrate the description stated above.



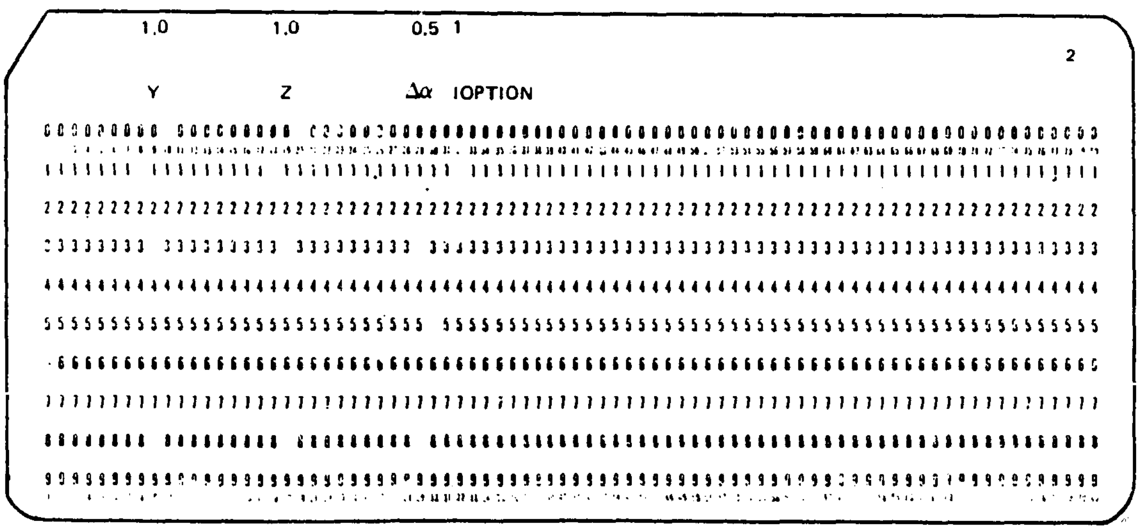


Figure 4.

NOTE: 1. The program user may include as many data sets as required in a single run of the program.

2. The values of all 12 input parameters must be punched on all data card sets.

EXAMPLE AND DESCRIPTION OF DATA

A typical example of the program and detailed description of the output data is as follows:

Example: Design a holographic diffraction grating that simultaneously corrects for astigmatism, coma, and the first spherical aberration term at 5000 Å for a Rowland circle spectrograph. The grating has 1200 L/mm and a 1.0 meter radius of curvature. Determine the performance of the holographic grating and equivalent conventional grating throughout the wavelength range 4500 Å to 9000 Å at 500 Å intervals.

Solution: Data cards are punched using the data supplied in the example and punched in the order listed below:

First Card

1. R = 1000 mm
2. N = 1200 L/mm
3. λ_o = 4579.3 Å
4. λ_c = 5000 Å
5. λ_U = 9000 Å
6. λ_L = 4500 Å
7. $\Delta\lambda$ = 500 Å
8. K = +1.0

Second Card

9. Y = 1.0
10. Z = 1.0
11. $\Delta\alpha = 0.5°$
12. IOPTION = 1

The output data for the example cited is shown in Figure 5. Output data for only one of the angles of incidence will be presented for the purpose of illustration.

A detailed description of the output data for simultaneously correcting astigmatism, coma, and the first spherical aberration term at 5000 Å is as follows:

*************************************** GRATING PARAMETERS ****

1 LAMDA= 5000.00 ANG ALFA= 30.7666 DEG BETA= 5.0749 DEG GAMA= 29.9935 DEG DELTA= -2.8429

2 AT THE THE CORRECTING WAVELENGTH= 5000.00 THE ABBERRATIONS ARE AS FOLLOWS:-

3 LAMDA	A1	A2	C1	C2	S1	S2	S3
4 5000.0	0.0	0.316973D-04	0.0	0.152375D-04	0.316973D-04	0.611084D-02	-0.300787D-02

5 ********************** GRATING PERFORMANCE ****************

6 HOLOGRAPHIC:...

7 LAMDA	A1	A2	C1	C2	S1	S2	S3
4500.0	0.0	0.242223D-01	0.0	0.175398D-01	0.242223D-01	0.511699D-01	0.107485D-01
5000.0	0.0	0.316973D-04	0.0	0.152375D-04	0.316973D-04	0.611084D-02	-0.300787D-02
5500.0	0.0	-0.167732D-01	0.0	-0.155338D-01	-0.167732D-01	-0.308045D-01	-0.975755D-02
6000.0	0.0	-0.258652D-01	0.0	-0.276076D-01	-0.258652D-01	-0.578552D-01	-0.987015D-02
6500.0	0.0	-0.267159D-01	0.0	-0.344253D-01	-0.267159D-01	-0.721124D-01	-0.401770D-02
7000.0	0.0	-0.185462D-01	0.0	-0.337530D-01	-0.185462D-01	-0.689294D-01	0.664532D-02
7500.0	0.0	-0.243867D-03	0.0	-0.226364D-01	-0.243867D-03	-0.410382D-01	0.201533D-01
8000.0	0.0	0.297695D-01	0.0	0.302645D-02	0.297695D-01	0.230676D-01	0.331204D-01
8500.0	0.0	0.737600D-01	0.0	0.492164D-01	0.737600D-01	0.142145D 00	0.395676D-01
9000.0	0.0	0.135067D 00	0.0	0.125127D 00	0.135067D 00	0.348134D 00	0.285334D-01
9500.0	0.0	0.218813D 00	0.0	0.245781D 00	0.218813D 00	0.698762D 00	-0.211611D-01
10000.0	0.0	0.333324D 00	0.0	0.437570D 00	0.333324D 00	0.130705D 01	-0.153539D 00

8 CONVENTIONAL:....

9 LAMDA	A1	A2	C1	C2	S1	S2	S3
4500.0	0.0	0.305346D 00	0.0	0.181322D 00	0.305346D 00	0.521213D 00	0.197413D 00
5000.0	0.0	0.312392D 00	0.0	0.181997D 00	0.312392D 00	0.528381D 00	0.204397D 00
5500.0	0.0	0.326823D 00	0.0	0.184645D 00	0.326823D 00	0.543693D 00	0.218398D 00
6000.0	0.0	0.348967D 00	0.0	0.190769D 00	0.348967D 00	0.568870D 00	0.239016D 00
6500.0	0.0	0.379352D 00	0.0	0.202150D 00	0.379352D 00	0.606839D 00	0.265608D 00
7000.0	0.0	0.418758D 00	0.0	0.221020D 00	0.418758D 00	0.662250D 00	0.297012D 00
7500.0	0.0	0.468296D 00	0.0	0.250335D 00	0.468296D 00	0.742368D 00	0.331260D 00
8000.0	0.0	0.529546D 00	0.0	0.294196D 00	0.529546D 00	0.855701D 00	0.364968D 00
8500.0	0.0	0.604772D 00	0.0	0.358584D 00	0.604772D 00	0.103000D 01	0.392156D 00
9000.0	0.0	0.697315D 00	0.0	0.452592D 00	0.697315D 00	0.128822D 01	0.401862D 00
9500.0	0.0	0.812297D 00	0.0	0.591544D 00	0.812297D 00	0.169108D 01	0.372908D 00
10000.0	0.0	0.958044D 00	0.0	0.801632D 00	0.958044D 00	0.235159D 01	0.261270D 00

****

Figure 5.

Line 1: Shows the correcting wavelength LAMDA = λ_c, angle of incidence ALFA = α, diffracted wavelength BETA = β, recording angle GAMA = γ and recording angle DELTA = δ.

Line 2: Self-explanatory.

Line 3: Shows the symbols for the wavelength and each aberration. The symbols for the aberrations have been defined in the text.

Line 4: Shows the correcting wavelength and values for each aberration at the correcting wavelength.

Line 5: Self-explanatory.

Line 6: Indicates that the holographic grating has been evaluated.

Line 7: Shows the titles of wavelength = LAMDA and the aberrations A_1, A_2, C_1, C_2, S_1, S_2 and S_3. The table shows the values of each aberration as a function of wavelength.

Line 8: Indicates that Line 9 and the corresponding table are for the evaluation of the equivalent conventional grating. The equivalent conventional grating is defined as having the same groove frequency and radius of curvature as the holographic grating. However, the conventional grating cannot correct aberrations. Note the reduction in aberration values as a function of wavelength as compared to the conventional grating. For example, at 5000 Å the value of astigmatism A_2 for the holographic grating is 0.316973×10^{-4} and that for the conventional grating is 0.31292. This shows that astigmatism is significantly reduced by a factor of 10^4 for the holographic grating at 5000 Å. Note that C_2 and S_1 are also reduced by the same order of magnitude. The remaining spherical aberration terms are also reduced by a factor of 10^2 for the same wavelength. Also note that the aberrations increase for decreasing and increasing wavelengths about the correcting wavelength at 5000 Å. However, the increase in aberrations remains less than that of the equivalent conventional grating.

In summary, the theory and basic equations have been presented to design concave spherical holographic reflecting diffraction gratings that are corrected to zero at specified wavelengths at or above the laser recording wavelength. A numerical analysis shows that there are specific angles of incidence based on the selected groove frequency and correcting wavelength that simultaneously corrects the aberrations A_2, C_2 and S_1. A computer program has been developed so that application of the theory may be applied to practical spectroscopic instrument design requirements for space and ground based laboratory applications.

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DESIGN OF ABERRATION CORRECTED HOLOGRAPHIC TOROID GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

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DESIGN OF ABERRATION CORRECTED HOLOGRAPHIC TOROID GRATINGS FOR SEYA-NAMIOKA TYPE MONOCHROMATORS

Part I: Minimization of Aberrations For Desired Wavelength Range

A. J. Caruso
M.S. Bhatia

Seya-Namioka type monochromators are designed such that wavelength selection is obtained by rotating a concave reflecting grating about its vertical axis. Diffracted image focussing is achieved by one optical element; normally a concave spherical reflecting diffraction grating. The angle of deviation, defined as the angle between the entrance and exit slits relative to the vertex of the grating, is a fixed value, normally 70°. At this fixed value most of the optical aberrations are reasonably acceptable except for severe astigmatism which is caused by the mechanically ruled concave spherical grating. With the advent of ruling holographic aberration corrected concave spherical reflecting diffraction gratings, it has become possible to design Seya-Namioka type monochromators such that astigmatism or coma may be corrected to zero at specified wavelengths or minimized over a desired wavelength range (ref, *1, 2, 3, 6*). These holographic grating designs have resulted in a significant improvement for the output efficiency of Seya-Namioka monochromators for wavelengths longer than 100 nm. However, for spherical concave gratings with angles of deviation greater than 70° holographic grating theory shows that aberration correction cannot be achieved for wavelengths shorter than 80 nm. Further, at 70° angle of deviation the output efficiency is also decreased because grating coating materials reflectivity is significantly reduced at wavelengths below 10.5 nm.

In order to over come this problem, we have substituted the toroid geometry for the grating blank in place of the concave spherical geometry. (reference 5) The major advantage of the toroid geometry is that astigmatism can be eliminated at specified wavelengths and also dramatically minimized over a wide wavelength range by properly determining the correct toroid vertical radius of curvature and horizontal radius of curvature as a function of the angle of incidence and the required holographic ruling geometry. Another advantage is that at larger incident angles the reflectivity of the same grating coating material increases at wavelengths less than 10.5 nm.

The purpose of this report is to present the theory and design equations for holographically ruled toroidal diffraction gratings that minimize aberrations for Seya-Namioka type monochromators with angles of deviation larger than or equal to the normal 70° for wavelengths shorter than 100 nm.

This report is divided into four sections. Section 1 presents the theory and design equations for designing aberration corrected holographic toroidal gratings. Two methods have been developed: the general method requires that the instrumental parameters be related only to the holographic toroid grating design. The second method is called the modified method. This method requires that the instrumental parameters be the same for both the conventional and holographic toroidal gratings. The modified method therefore designs such that the holographically ruled toroidal grating is interchangeable with the conventionally ruled grating providing they have the same groove frequency, and radius of curvatures R and ρ_t.

Section 2 presents a description of the computer program. The program has been developed such that for a given groove frequency and wavelength range, the optimum instrumental and holographic ruling parameters are determined for the toroidal concave grating. The program also displays the performance of the holographic toroidal grating and equivalent conventional toroidal grating, as a function of wavelength relative to optical aberrations such as astigmatism, coma, and spherical aberrations. Section 3 presents the input data, definition of terms and data card description. Section 4 presents an example for using the program and describes in detail the output data.

Section 1
Theory and Basic Equations for Designing Holographic Toroidal Concave Gratings

A toroid is produced when a circle is rotated about an axis which lies in the plane of the circle but does not pass through the midpoint of the circle (Fig. 1). Figure (1) also shows a section (toroidal grating blank) cut out of the toroid for which there are two radii of curvatures: a long horizontal

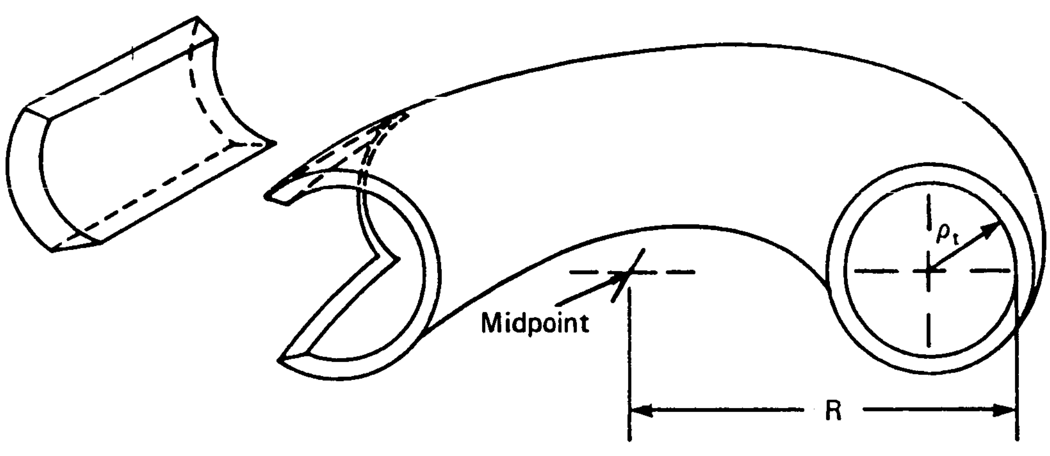

Figure 1. Schematic diagram of a toroid. R and ρ_t are the radii of the toroidal surface. Cut out section is typical of a toroid grating blank

radius R and a short vertical radius ρ_t. If $\rho_t = R$, then a spherical concave surface will be generated; ie, when the axis of rotation passes through the midpoint of the circle. As a result, all inferences which are valid for the toroid are also valid for the sphere when $\rho_t = R$.

We now proceed with the theory and basic equations for designing holographic toroidal gratings with the above concept in mind.

Figure (2) shows a toroidal grating blank in an optical schematic diagram which defines a rectangular coordinate system. Let the origin be at vertex O of the concave toroid grating blank which has a horizontal radius of curvature R and a vertical radius of curvature ρ_t. Let the x-axis be defined by O and two coherent point light sources C and D which are used to produce the interference fringes on the concave toroidal blank surface. Points A, P, and B are self luminus points on the entrance slit, a point on the grating and a point at the focused diffracted image from P at wavelength λ in the m^{th} order respectively. A knowledge of the geometrical optical system of Figure 2 leads to writing the aberrant optical light path function F for the conventional grating as

$$F = AP + PB + mn\,\lambda \tag{1}$$

where n is the groove frequency, m is the diffracted order and λ is the diffracted wavelength.

When a grating substrate coated with a photoresist layer is illuminated by coherent spherical wavefronts originating from points C and D, grooves are recorded and formed after development in the photoresist in response to the interference fringes produced at the site of the grating surface. The interference fringes are formed according to equation

$$n\lambda_o = [(CP) - (DP)] - [(CO) - (DO)] \tag{2}$$

where n is the groove frequency and λ_o is the laser wavelength radiation.

Substituting equation (2) into equation (1) gives the aberrant optical light path function

$$F = AP + PB + \frac{m\lambda}{\lambda_o}[(CP - DP) - (CO - DO)] \tag{3}$$

for the holographic grating. The terms on the right side of F in equation (3) are derived based on the coordinate system described in Figure (2). By substituting the trignometric terms for the toroid and other required terms, in equation (3), the following aberrant optical light path function F is derived after a power series expansion is performed.

$$\begin{aligned} F = F_{000} &+ WF_{100} + LF_{011} + \tfrac{1}{2}W^2F_{200} + \tfrac{1}{2}L^2F_{020} \\ &+ \tfrac{1}{2}W^3F_{300} + \tfrac{1}{2}WL^2F_{120} + WLF_{111} \\ &+ 1/8\,W^4F_{400} + \tfrac{1}{4}W^2L^2F_{220} + 1/8\,L^4F_{040}\ \tfrac{1}{4}WL^2F_{202} \\ &+ \tfrac{1}{4}L^2F_{022} + \tfrac{1}{2}L^3F_{031} + \tfrac{1}{2}W^2LF_{211} + \dots \end{aligned} \tag{4}$$

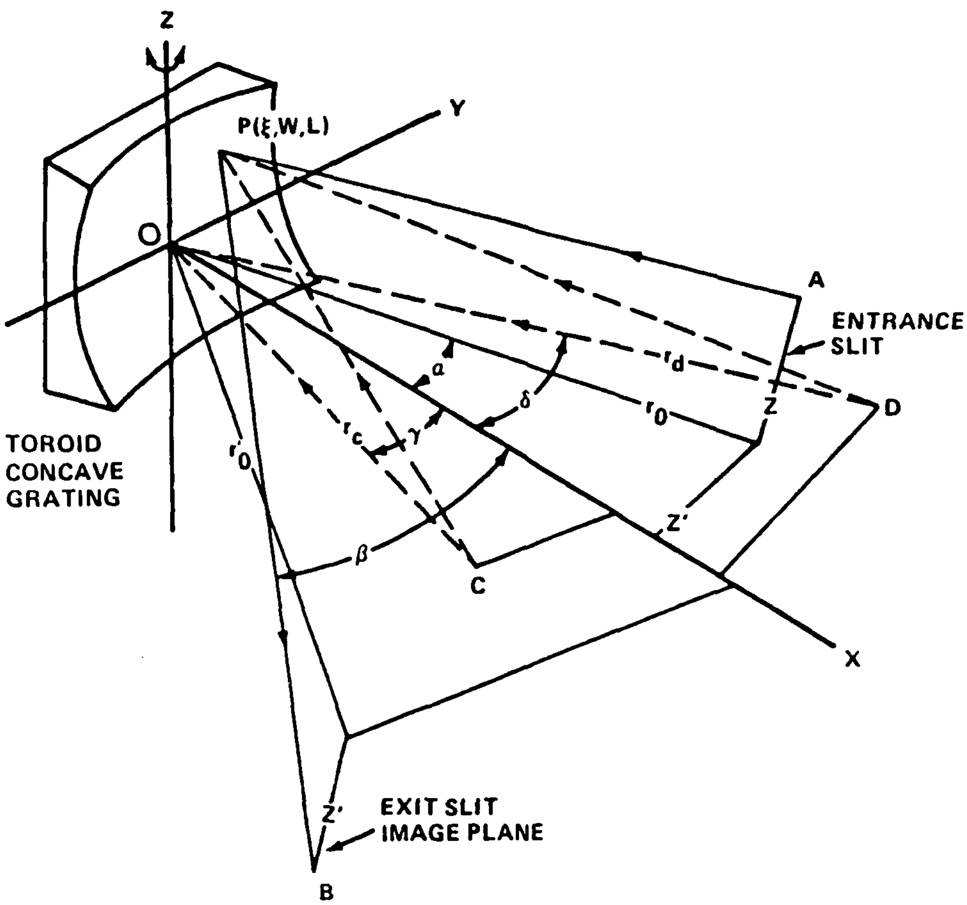

Figure 2. Schematic diagram showing the geometry for recording the holographic grating. The instrumental and recording parameters are defined as follows:

Instrument Parameters

- r_0 is the object distance from the entrance slit to the center of the grating.
- r_0' is the image distance from the exit slit to the center of the grating.
- α is the angle of incident radiation relative to the normal of the grating.
- β is the diffracted image angle relative to the normal of the grating.
- A is the entrance slit position and B is the exit slit position.

Recording Parameters

- r_C is the distance of recording point source C to the center of the grating.
- r_D is the distance of the recording point source D to the center of the grating.
- δ is the recording angle for positioning point source D relative to the normal of the grating.
- γ is the recording angle for positioning point source C relative to the normal of the grating.

and

$$F_{ijk} = M_{ijk} + \left(\frac{m\lambda}{\lambda_o}\right) H_{ijk} \tag{5}$$

where the subscripts ijk of F_{ijk} are exponents of $W^i L^j Z^k$ except for F_{0c0}.

The terms M_{ijk} and H_{ijk} are defined in terms of the function f_{ijk} as follows

$$\begin{aligned} M_{ijk} &= f_{ijk}(\rho, \alpha) + f_{ijk}(\rho', \beta) \\ H_{ijk} &= f_{ijk}(\rho_c, \gamma) - f_{ijk}(\rho_D, \delta) \end{aligned} \tag{6}$$

for ijk = (200) and (300)

and

$$\begin{aligned} M_{ijk} &= f_{ijk}(\rho, q, \alpha) + f_{ijk}(\rho', q, \beta) \\ H_{ijk} &= f_{ijk}(\rho_c, q, \gamma) + f_{ijk}(\rho_D, q, \delta) \end{aligned} \tag{6a}$$

for ijk = (020) and (120)

$$\begin{aligned} M_{ijk} &= M_{020} - (-1)^{½ i} [f_{ijk}(\rho, \alpha) + f_{ijk}(\rho', \beta)] \\ H_{ijk} &= H_{020} - (-1)^{½ i} [f_{ijk}(\rho_c, \gamma) - f_{ijk}(\rho_D, \delta)] \end{aligned} \tag{7}$$

for ijk = (400)

and

$$\begin{aligned} M_{ijk} &= M_{020} - (-1)^{½ i} [f_{ijk}(\rho, q, \alpha) + f_{ijk}(\rho', q, \beta)] \\ Hijk &= M_{020} - (-1)^{½ i} [f_{ijk}(\rho_c, q, \gamma) - f_{ijk}(\rho_D, q, \delta)] \end{aligned} \tag{7a}$$

for ijk = (220) and (040)

where the expressions for the conventional toroid grating are

$$f_{200}(\rho, \alpha) + f(\rho', \beta) = \cos\alpha(\rho\cos\alpha - 1) + \cos\beta(\rho'\cos\beta - 1) \tag{8a}$$

$$f_{020}(\rho, q, \alpha) + f(\rho', q, \beta) = \rho - q\cos\alpha + \rho' - q\cos\beta \tag{8b}$$

$$f_{300}(\rho, \alpha) + f(\rho', \beta) = \rho\sin\alpha\cos\alpha(\rho\cos\alpha - 1) + \rho'\sin\beta\cos\beta(\rho'\cos\beta - 1) \tag{8c}$$

$$f_{120}(\rho, q, \alpha) + f(\rho' q, \beta) = \rho\sin\alpha(\rho - q\cos\alpha) + \rho'\sin\beta(\rho' - q\cos\beta) \tag{8d}$$

$$f_{400}(\rho, \alpha) + f_{400}(\rho', \beta) = \rho - \cos\alpha - \rho\cos\alpha(\rho\cos\alpha - 1)[\cos\alpha(\rho\cos\alpha - 1) - 4\rho\sin^2\alpha] \tag{8e}$$

$$+\rho' - \cos\beta - \rho'\cos\beta\,(\rho'\cos\beta-1)\,[\cos\beta\,(\rho'\cos\beta-1) - 4\,\rho'\sin^2\beta]$$

$$f_{220}(\rho, q, \alpha) + f_{220}(\rho', q, \beta) = q\,(\rho\sin^2\alpha - \cos\alpha) + \rho^2\cos\alpha$$
$$+ (3\rho^2\sin^2\alpha - \rho^2)(\rho - q\cos\alpha) \tag{8f}$$
$$+ q\,(\rho'\sin^2\beta - \cos\beta) + \rho'^2\cos\beta + (3\rho'^2\sin^2\beta - \rho'^2)\,(\rho' - q\cos\beta)$$

$$f_{040}(\rho, q, \alpha) + f_{040}(\rho', q, \beta) = q^2(\rho - q\cos\alpha) - \rho(\rho - q\cos\alpha)^2$$
$$+ q^2(\rho' - q\cos\beta) - \rho'(\rho' - q\cos\beta)^2 \tag{8g}$$

and the expressions for the holographic contribution are:

$$f_{200}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = \cos\gamma(\rho_c\cos\gamma - 1) - \cos\delta\,(\rho_D\cos\delta - 1) \tag{8h}$$

$$f_{020}(\rho_c, q, \gamma) - f_{020}(\rho_D, q, \delta) = \rho_c - q\cos\gamma - \rho_D - q\cos\delta \tag{8i}$$

$$f_{300}(\rho_c, \gamma) - f_{300}(\rho_D, \gamma) = \rho_c\sin\gamma\cos\gamma\,(\rho_c\cos\gamma - 1) - \rho_D\sin\delta\cos\delta\,(\rho_c\cos\delta - 1) \tag{8j}$$

$$f_{120}(\rho_c, q, \gamma) - f_{120}(\rho_c, q, \delta) = \rho_c\sin\gamma\,(\rho_c - q\cos\gamma) - [\rho_D\sin\delta\,(\rho_D - q\cos\delta)] \tag{8k}$$

$$f_{400}(\rho_c, \gamma) - f_{400}(\rho_D, \delta) = \rho_c \quad \cos\gamma - \rho_c\cos\gamma\,(\rho_c\cos\gamma - 1)$$
$$(\cos\gamma\,(\rho_c\cos\gamma - 1) - 4\,\rho_c\sin^2\gamma)$$
$$- [\rho_D - \cos\delta - \rho_D\cos\delta\,(\rho_c\cos\gamma - 1) \tag{8l}$$
$$(\cos\delta\,(\rho_c\cos\delta - 1) - 4\,\rho_c\sin^2\delta)$$

$$f_{220}(\rho_c, q, \gamma) - f_{220}(\rho_D, q, \delta) = q\,(\rho_c\sin^2\gamma - \cos\gamma) + \rho_c^2\cos\gamma$$
$$+ (3\rho_c^2\sin^2\gamma - \rho_c^2)(\rho_c - q\cos\gamma) \tag{8m}$$
$$- [q(\rho_D\sin^2\delta - \cos\delta) + \rho_D^2\cos\delta + (3\rho_D^2\sin^2\delta - \rho_D^2)(\rho_D - q\cos\delta)]$$

$$f_{040}(\rho_c, q, \gamma) - f_{040}(\rho_D, q, \delta) = q^2(\rho_c - q\cos\gamma) - \rho_c(\rho_c - q\cos\gamma)^2$$
$$- [q^2(\rho_D - q\cos\delta) - \rho_D(\rho_D - q\cos\delta)^2] \tag{8n}$$

where

$$\rho = \frac{R}{r},\ \rho' = \frac{R}{r'},\ \rho_c = \frac{R}{r_c},\ \rho_D = \frac{R}{r_D} \tag{9}$$

and $q = \frac{R}{\rho_t}$ where R is the horizontal radius and ρ_t is the vertical radius of the toroid.

The term F_{100} in equation 4 is the well known grating equation and is given as

$$m\lambda = \sigma (\sin \alpha + \sin \beta) \qquad (10)$$

for the principal ray, the ray originating from the center of the entrance slit and diffracted from O at an angle β. In order to holographically rule the grating with the required groove frequency, the effective grating constant is defined as

$$\sigma = \frac{\lambda o}{\sin \delta - \sin \gamma} \qquad (11)$$

where $\delta > \gamma$. γ and δ are the recording angles.

Note that the number of grooves per unit length is $n = \frac{1}{\sigma}$.

The individual expressions for equations (8a) thru (8n) have physical significance as to the formation and imperfections of the diffracted image. The expressions control the various conditions for the foci and image deficiencies in the following order; 8a and 8h govern the primary focusing condition on the Rowland Circle, 8b and 8i determine the amount of astigmatism relative to the diffracted image, 8c, 8j, 8d, and 8k Coma, 8e and 8l higher order focusing condition on the Rowland Circle and 8f, 8g, 8m and 8n the toric aberrations. It is interesting to note that when one compares these expressions of the toroid with those for the equation of a sphere Ref (1), there are some expressions that are identical for both. (toroid & sphere). For example, all the expressions which do not include q are identical with those expressions for the sphere. It is only those expressions that involve q that account for the difference between the two gratings. Note that the difference between the two gratings vanishes when ρ_t = R.

Minimization of Aberrations

The theory described up to this point has been presented for the general case. We now apply the general theory to a specific application: The Seya-Namioka monochromator. This type of monochromator has a single reflecting and wavelength dispersing element; the grating. Wavelength selection is achieved by rotating the grating about the vertical axis at the front surface of the center of the grating. The basic instrumental parameters for this type monochromator are defined as follows; see fig *3*.

$$r_o, \bar{r}'_o = \text{constant}, \; 2K = \alpha_o - \beta_o = \text{constant}$$
$$\alpha_o = K + \theta, \; \beta_o = \theta - K \qquad (12)$$

where r_o is the distance from the center of the extrance slit to O and $\bar{r}'_o$ is the distance from O to the center of the exit slit. 2K is the angle of deviation AOB and θ is the angle of grating rotation measured from the bisector of the angle 2K and has the same sign as the spectral order m.

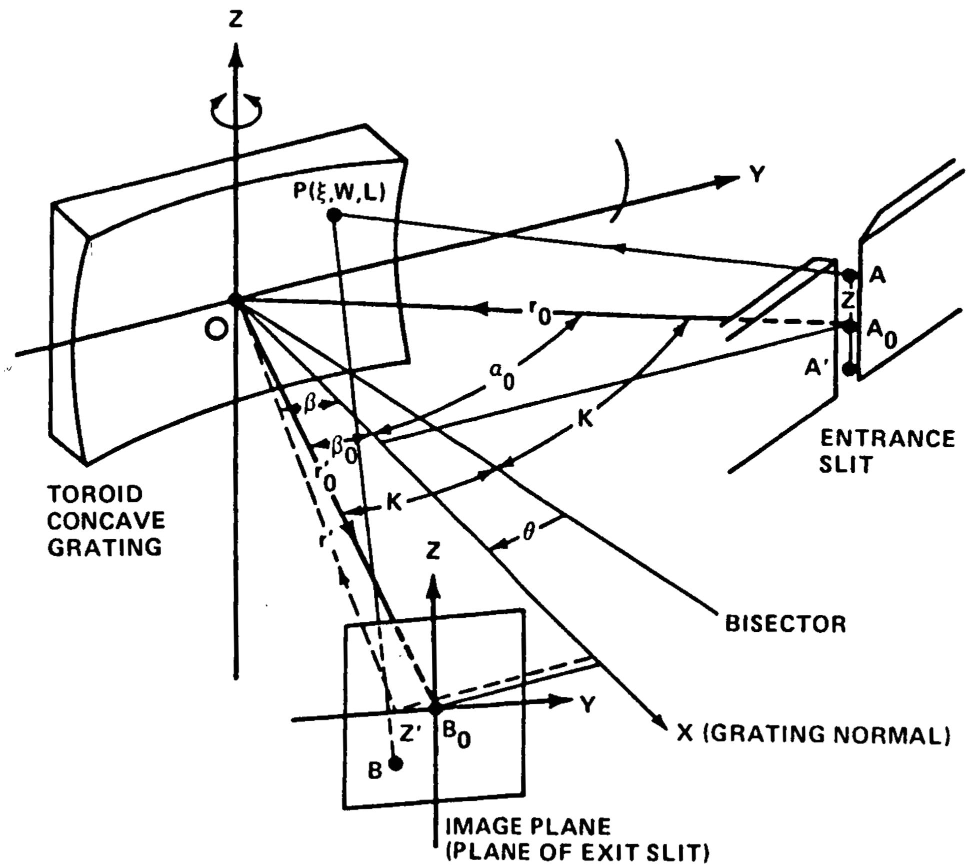

Figure 3. Schematic diagram of the optical system for Seya-Namioka monochromator

Under conditions (12), the relation between θ and λ is given by

$$\lambda = \left(\frac{2\sigma}{m}\right) \cos k \sin \theta \tag{13}$$

In order to reduce the aberrations in the Seya-Namioka monochromator, we denote the function F_{ijk} for the ray AOB by F_{ijK}. We then minimize the function

$$\overline{F}_{ijk}\,(\bar{\rho}, \bar{\rho}', q, \theta, K, A_{ijk}) = \overline{M}_{ijk} + \left(\frac{m\lambda}{\lambda_o}\right) H_{ijk} = \overline{M}_{ijk} + A_{ijk}\,(\sin \alpha_o + \sin \beta_o) \tag{14}$$

where $i + j + k \geqslant 2$ over a predetermined scanning range, $\theta \leqslant \theta \leqslant \theta_2$ or $\lambda_1 \leqslant \lambda \leqslant \lambda_2$ where

$$\bar{\rho} = \frac{R}{r_o}, \bar{\rho}' = \frac{R}{\bar{r}'} = \frac{R}{r_o'} \text{ and } q = \frac{R}{\rho_t} \tag{15}$$

$$A_{ijk} = \frac{H_{ijk}}{\sin \delta - \sin \gamma} = \left(\frac{\sigma}{\lambda_o}\right) H_{ijk} \tag{16}$$

and θ_1 and θ_2 are related to λ_1 and λ_2 through equation (13). This is equivalent to imposing on $\overline{F}_{ijk}$ the condition

$$I_{ijk} = \int_{\theta_1}^{\theta_2} \overline{F}^2_{ijk}\, d\theta = \text{minimum} \tag{17}$$

Determination of Instrumental Parameters $\bar{\rho}$, $\bar{\rho}'$, K, q and A_{200}

The optimum instrumental parameters are determined in such a way that equation (17) is satisfied for the horizontal focusing condition $\overline{F}_{200}$. This is accomplished by solving the following equations simultaneously,

$$\frac{\partial I_{200}}{\partial \bar{\rho}} = 0, \quad \frac{\partial I_{200}}{\partial \bar{\rho}'} = 0$$

$$\frac{\partial I_{200}}{\partial K} = 0, \quad \frac{\partial I_{200}}{\partial A_{200}} = 0 \tag{18}$$

With the values of $\bar{\rho}$, $\bar{\rho}'$ and K determined, we proceed to determine the value of q, where $q = \frac{1}{P}$.

P has been derived by Greiner and Schaffer (ref 4) as

$$P = \frac{2 \cos K \,(\sin(\theta_2 - \theta_1))}{(\bar{\rho} + \bar{\rho}')\,(\theta_2 - \theta_1)} \tag{18a}$$

where K is the half angle between the entrance and exit slits relative to the vertex of the grating, θ_2 and θ_1 are the limits of the angular rotation of the grating and

$$\bar{\rho} = \frac{R}{r_o} \text{ and } \bar{\rho}' = \frac{R}{r_o'}.$$

q is a very important parameter in that it determines the optimum geometry of the toroid grating for the desired wavelength range. Since R is a selected value and the optimum q has been determined by (18a), then the vertical radius of curvature of the toroid grating may be calculated using equation

$$q = \frac{1}{P} = \frac{R}{\rho_t} \tag{18b}$$

When the optimum values of $\bar{\rho}$, $\bar{\rho}'$, K and q are determined, then each one of the integrals I_{ijk} with $i + j + k \geqslant 2$ becomes a function only of A_{ijk}. Those values of A_{ijk}'s which satisfy equation (17) are calculated from equation

$$\frac{\partial I_{ijk}}{\partial A_{ijk}} = 2\int_{\theta_1}^{\theta_2} \overline{F}_{ijk} \cdot \frac{\partial F_{ijk}}{\partial A_{ijk}} \, d\theta = 0 \tag{19}$$

where

$$A_{ijk} = [B_{ijk}(\theta_2) - B_{ijk}(\theta_1)] / [2(\theta_1 - \theta_2) - (\sin 2\theta_2 - \sin 2\theta_1 0)] \cos K \tag{20}$$

and

$$\begin{aligned} B_{200}(\theta) = (\overline{\rho}/3[&\cos\theta + \cos(\theta + K)\cos(2\theta + K) \\ &+ 3\sin(\theta + K)\sin K] \\ &+ (\overline{\rho}'/3)[\cos\theta + \cos(\theta - K)\cos(2\theta - K) \\ &- 3\sin(\theta - K)\sin K] - \cos 2\theta \cos K \end{aligned} \tag{21}$$

$$B_{020}(\theta) = 2(\overline{\rho} + \overline{\rho}')\cos\theta - q\cos 2\theta \cos K \tag{22}$$

$$\begin{aligned} B_{300} = (\overline{\rho}/4)^2 &[\sin[4\theta + 3K] - 4\cos 2(\theta + K)\sin K - 4\theta\cos K] \\ &+ (\overline{\rho}'/4)^2 [\sin[4\theta - 3K] + 4\cos 2(\theta - K)\sin K - 4\theta\cos K] \\ &+ (\overline{\rho}/6)[3\sin(\theta + 2K] - \sin(3\theta + 2K)] \\ &+ (\overline{\rho}'/6)[3\sin(\theta - 2K) - \sin(3\theta - 2K)] \end{aligned} \tag{23}$$

$$\begin{aligned} B_{120}(\theta) = (\tfrac{1}{2}\rho)2 &[\sin(2\theta + K) - 2\theta\cos K] \\ &+ (\tfrac{1}{2}\overline{\rho}')^2 [\sin(2\theta - K) - 2\theta\cos K] \\ &+ \frac{q\overline{\rho}}{6}[3\sin(\theta + 2K) - \sin(3\theta + 2K)] \\ &+ \frac{q\overline{\rho}'}{6}[3\sin(\theta - 2K) - \sin(3\theta - 2K)] \end{aligned} \tag{24}$$

and so on.

<u>Determination of the Recording Parameters ρ_c, ρ_d, γ and δ and Minimization of Astigmatism and Coma</u>

The recording parents depend upon the aberrations to be minimized. With a predetermined effective grating constant and wavelength range, the following equations are solved simultaneously for minimizing astigmatism and one coma-type aberration.

$$\sin\delta - \sin\gamma = \frac{\lambda o}{\sigma}$$

$$f_{200}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = (\lambda o/_\sigma) A_{200}$$

$$f_{020}(\rho_c, q, \gamma) - f_{020}(\rho_D, q, \delta) = (\lambda o/_\sigma) A_{020} \qquad (25)$$

$$f_{300}(\rho_c, \gamma) - f_{30}(\rho_D, \delta) = (\lambda o/_\sigma) A_{300}$$

and for minimizing coma-type aberrations

$$\sin\delta - \sin\gamma = \frac{\lambda}{\sigma}$$

$$f_{200}(\rho_c, \gamma) - f_{200}(\rho_D, \delta) = (\lambda o/_\sigma) A_{200}$$

$$f_{300}(\rho_c, \gamma) - f_{300}(p_D, \delta) = (\lambda o/_\sigma) A_{300} \qquad (26)$$

$$f_{120}(\rho_c, q, \gamma) - f_{120}(\rho_D, q, \delta) = (\lambda o/_\sigma) A_{120}$$

Before making any attempt to solve equations (25) or (26) it is necessary to investigate the conditions under which equations (25) or (26) can have real solutions for ρ_c and ρ_D because H_{300} and H_{120} are quadratic in ρ_c and ρ_D and their values depend on A_{300} and A_{120} and therefore on the values of θ_2 in I_{300} and I_{120}. The condition may be stated in such a way that two quadratic equations of ρ_c or ρ_D resulting from equations (25) and (26) should not have imaginary roots. To fulfill this condition, A_{300} and A_{120} must satisfy the equation

$$b^2 - 4ac \geqslant O \qquad (27)$$

where for A_{300}

$$a = (\sin\delta\cos^2\gamma - \sin\gamma\cos^2\delta)\cos^2\gamma$$

$$b = [2\rho\cos\gamma\sin\delta + \sin(\delta-\gamma)\cos\delta]\cos\gamma \qquad (28)$$

$$c = \rho(\rho + \cos\gamma)\sin\delta + A_{300}\cos^2\delta(\sin\delta - \sin\gamma)$$

and for A_{120}

$$a = \cos^4 \gamma \sin \delta - \sin \gamma \cos^4 \delta$$

$$b = [2\rho \cos \gamma \sin \delta + \sin(\delta - \gamma) \cos^3 \delta] \cos \gamma$$

$$c = \rho(\rho \sin \delta + \cos^3 \delta) \sin \delta + A_{120} \cos^4 \delta (\sin \delta - \sin \gamma) \tag{29}$$

$$\rho = A_{200}(\sin \delta - \sin \gamma) + \cos \gamma - \cos \delta.$$

when condition (27) is satisified, then ρ_c and ρ_D are solutions to equations (25) and (26).

Up to this point, we have been describing the general method of designing aberration corrected holographic toroid gratings for Seya-Namioka type monochromators which are not interchangeable with conventional toroidal gratings. We will now deal with the design method where both types of gratings are interchangeable.

Modified Method

The modified method of designing holographic toroidal gratings for the Seya-Namioka monochromator has a practical advantage in that it may now be designed so that it is interchangeable with the conventionally ruled toroidal grating having the same groove frequency and radius of curvatures R and ρ_t. This is possible provided the same instrumental constants $\bar{\rho}$, $\bar{\rho}'$, q and K used for the conventionally ruled gratings are used to design the holographic toroidal grating. The instrumental constants for the conventional toroidal grating are determined by solving the

equation $$I_{200} = \int_{\theta_1}^{\theta_2} \overline{M}_{200}^2 \, d\theta = \text{minimum}$$

or

$$\frac{\partial I_{200}}{\partial \bar{\rho}} = O, \quad \frac{\partial I_{200}}{\partial \rho'} = O$$

and

$$\frac{\partial I_{200}}{\partial K} = O \tag{30}$$

The design equations given by equations (17)-(26) must be modified in part in order to accommodate condition (30). The modification required is to replace equation (18) with equation (30) and equation (20) with (ijk) = (200) and the rest of the procedure remains the same.

The design of toroidal holographic gratings and optical systems for Seya-Namioka monochromators have been presented. Design equations for minimizing aberrations such as astigmatism and coma have been derived. By now, you must have observed the the design equations for concave toroid gratings are very similar to the design equations for concave spherical gratings. In fact, if the parameter q has a value of one; ie $\rho_t = R$, then the toroidal equations are identical to those equations for the sphere. The advantage of the concave toroid grating relative to the concave spherical grating is that astigmatism can be minimized for larger angles of incidence and at shorter wavelengths where under the same geometrical conditions the concave spherical grating cannot.

Section 2

Section 1 described the theory of designing holographic concave toroidal gratings that minimize aberrations for a selected wavelength range. In this section, we will apply the theory and present a computer program that will calculate all the necessary parameters for using and ruling the holographic toroid grating for the Seya-Namioka monochromator.

Program Description:

The computer program consists of a main program and four subroutines. Fig (4) is a flow chart diagram of the program.

The purpose of the main program is to direct the flow of calculations depending upon which option is selected. If option LMN=2 is selected, then the optimum value of the instrumental parameter angle 2K will be calculated. However, if the program user chooses to specify an angle 2K as an input value, then option LMN=1 is used.

Two toroidal holographic grating design methods have been developed: the general method and the modified method. If the general method is chosen then the option called I ETA=1 is used. When using this option, all instrumental parameters are related only to the toroidal holographic grating. However, if the modified method is selected, then the option IETA=0 is used in the program. When using this option, all instrumental parameters calculated are the same for both the holographic and conventional gratings. This means that the holographic and conventional toroid gratings are interchangeable if they have the same groove frequency and radii of curvatures. (R and ρ_t). The difference is that the holographic toroid grating minimizes aberrations and the conventional toroid grating only reduces astigmatism. When the design method has been selected and the option has been decided upon, the following steps of calculation are performed:

Step A: Read input cards

Step B: Call INSTRM to calculate the optimum angle 2K, $\bar{\rho}$, $\bar{\rho}'$ and ρ_t. Then calculate B_{ijk} and A_{ijk} from equation (20) where LMN=2 or calculate the functions B_{ijk} and A_{ijk} using the selected input value for 2K when LMN=1.

Step C: Call ASTGMS to calculate the recording parameters ρ_c, ρ_D, γ and δ to minimize astigmatism ijk = (020) and one coma term ijk = (300).

Step D: Call COMA to calculate the recording parameters ρ_c, ρ_D, γ and δ to minimize coma aberrations ijk = (300) and ijk = (120).

Step E: Call PRFORM to display the numerical values of each aberration of the holographic toroid grating and compare with that of the equivalent conventional grating as a function of wavelength. Note that the program automatically calculates the recording parameters for both the minimization of astigmatism and coma. This feature was included in the program so that the program user may select which aberration minimization will best produce the optimum minimization for all aberrations through out the desired wavelength range.

The procedure stated above is supported by four subroutines.

Subroutine INSTRM

Subroutine INSTRM determines the optimum values of the instrumental parameters $\bar{\rho}$, $\bar{\rho}'$, 2K, and A_{200} by simultaneous solution of equation (18). A modified form of Newton's method is used to obtain the solution. With a knowledge of $\bar{\rho}$, $\bar{\rho}'$ and 2K the optimum vertical radius of curvature ρ_t for the toroid is calculated. After all the optimum instrumental parameters are determined, then the values of the B_{ijk} are calculated which in turn are used in equation (20) to determine the values of A_{ijk}'s. Note that if a prescribed input value of 2K were used, the selection of option LMN=1 would by-pass the optimization procedures when calculating the other instrumental parameters.

Subroutine ASTGMS

The purpose of this subroutine is to obtain the recording parameters such that astigmatism (ijk) = (020) and one coma term (ijk) = (300) are minimized over the given wavelength range $\lambda_1 \leqslant \lambda \leqslant \lambda_2$. This is achieved by simultaneous solution of equation (25). Before proceeding with the solution, it is first verified that the value of $N\lambda o$ is less than the maximum value of $|(\sin \delta - \sin \gamma)|$, namely 2. If not, an error message is printed stating "error, GAMA out of bounds." Now, if $N\lambda o$ is less than 2 then the values of a, b, and c of equation (28) or (29) are computed and the discriminate is checked to ensure that $b^2 - 4ac \geqslant 0$. The solutions of the quadratic equations are computed and checked to make sure that the positive value has been used, because the calculations show that one of the two roots $[(-b \pm \sqrt{(b^2 - 4ac)}/_{2a}]$ is always positive and the other is always negative. When the discriminate has been verified to be positive, then the optimum values of ρ_c, ρ_D, γ and δ are determined by the iterated solution of equation (25) using Newton's method.

Subroutine COMA

The purpose of this subroutine is to obtain the recording parameters such that the coma terms ijk = (300) and ijk = (120) are minimized for a given wavelength range $\lambda_1 \leqslant \lambda \leqslant \lambda_2$. This is achieved by a simultaneous solution of equation (26). We use the same procedure used in subroutine ASTGMS to verify that the discriminant is positive and then proceed to determine the optimum values ρ_c, ρ_D, γ, and δ by the iterated solution of equation (26) using Newton's method.

MAIN PROGRAM FLOW DIAGRAM

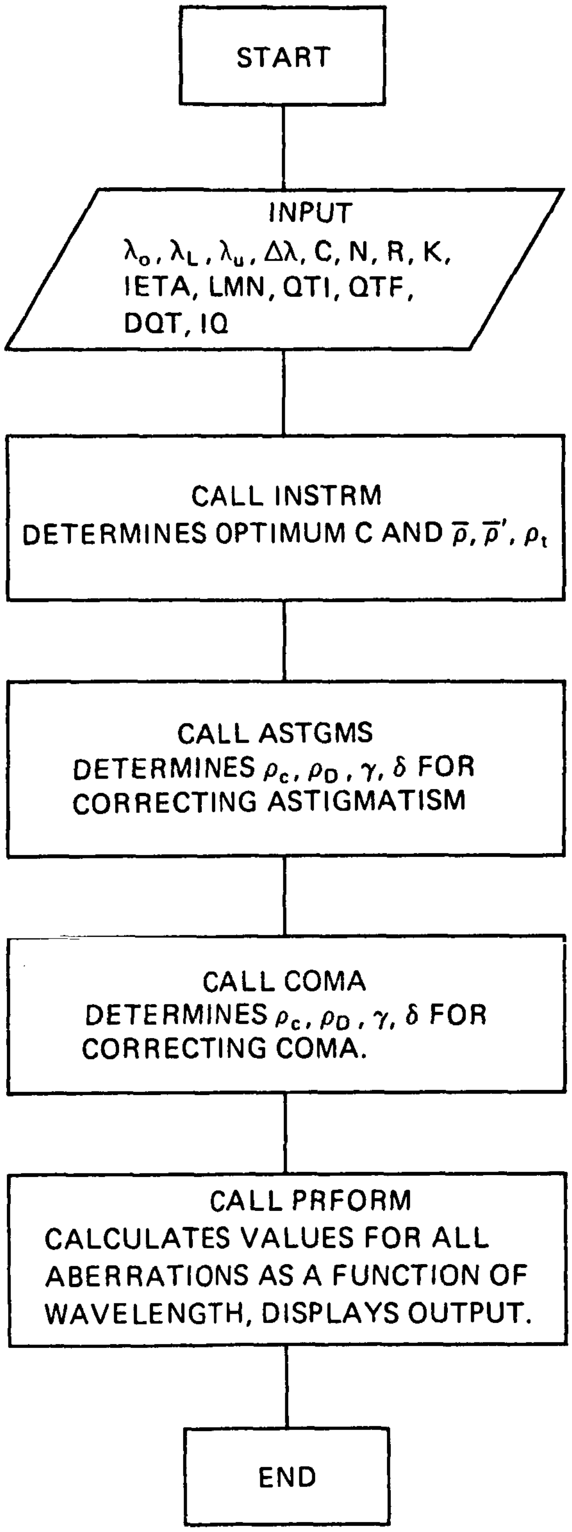

Figure 4. Main Program Flow Diagram

Subroutine PRFROM

This subroutine calculates the performance of the holographic toroid grating using the calculated instrumental and recording parameters and then displays the values of each aberration as a function of wavelength in the form of a table. The performance of a conventional (mechanically ruled) grating with the same groove frequency is also shown in the table for comparison.

Section 3. DATA SET AND DESCRIPTION OF DATA CARDS

This section discusses the input data required for a successful operation of the program.

(A) Data Set

The following parameters are required as input for the program.

1. λ_o = wavelength of recording laser light in angstroms.

2. λ_L = lower wavelength limit in angstroms.

3. λ_u = upper wavelength limit in angstroms.

4. $\Delta\lambda$ = wavelength interval in angstroms which aberrations will be displayed.

5. C = angle 2K (0.0 is used with option LMN=2).

6. N = groove frequency (number of lines per mm).

7. R = Radius of curvature in mm.

8. m = order of diffraction where m = ± 1, ± 2, etc.

9. IETA: Parameter specifying the grating design method. IETA = 1 specifies general method. IETA=0 specifies the modified method.

10. QTI = Initial value of the torus parameter q_i.

12. QFT = Final value of torus parameter q_f.

13. DQT = Interval at which the torus parameter Δq will change.

14. IQ = Parameter to specify the torus radius options.

    IQ=2; Torus parameter q is selected by user.

    IQ=1; Toroid radius ρ_t in mm is automatically computed

Note: If IQ=1 is selected, then QTI, QTF and DQT are NOT punched on the data card. The computer automatically bypasses these parameters and calculates the optimum q values and ρ_t. However the value 1 for IQ must be punched in the appropriate column on the card.

If IQ=2 is selected, then QTI, QTF, and DQT must be punched on the data card in the correct order. For this case, the computer will calculate the ρ_t based on the values selected for the range of q's desired.

(B) Description of Data Cards and Sample Data Cards

The first seven input parameters must be punched on the data cards in the order shown in (A) starting in column 1 in F10.1 format with ten columns reserved for each of the seven parameters and each parameter must include a decimal. The next three parameters are in I2 format starting in column 71. The parameters QTI, QTF, DQT, and IQ are punched on the second card in format F10.0 and I2 respectively. Fig (5) shows a typical two card data set to illustrate the above description.

Note: (1) The program user may include as many data cards for a single run as desired.

(2) The values of all 14 parameters must be punched for each additional set.

Section 4

This section presents a typical example for using the program and also describes the output data in detail.

Example: Determine the optimum instrumental and recording parameters for designing a concave toroid holographic grating for a Seya-Namioka monochromator that minimizes astigmatism or coma and has the following specifications:

1. Interchangeable with conventional concave toroid grating.
2. Groove frequency = 550 L/mm
3. R = 1,000 mm
4. Operating wavelength range = 0.0Å to 1600Å.
5. Order = −1
6. C = 142°

Solution:

(1) indicates that the modified method is used; IETA=0. (6) says that option LMN=1 is used.

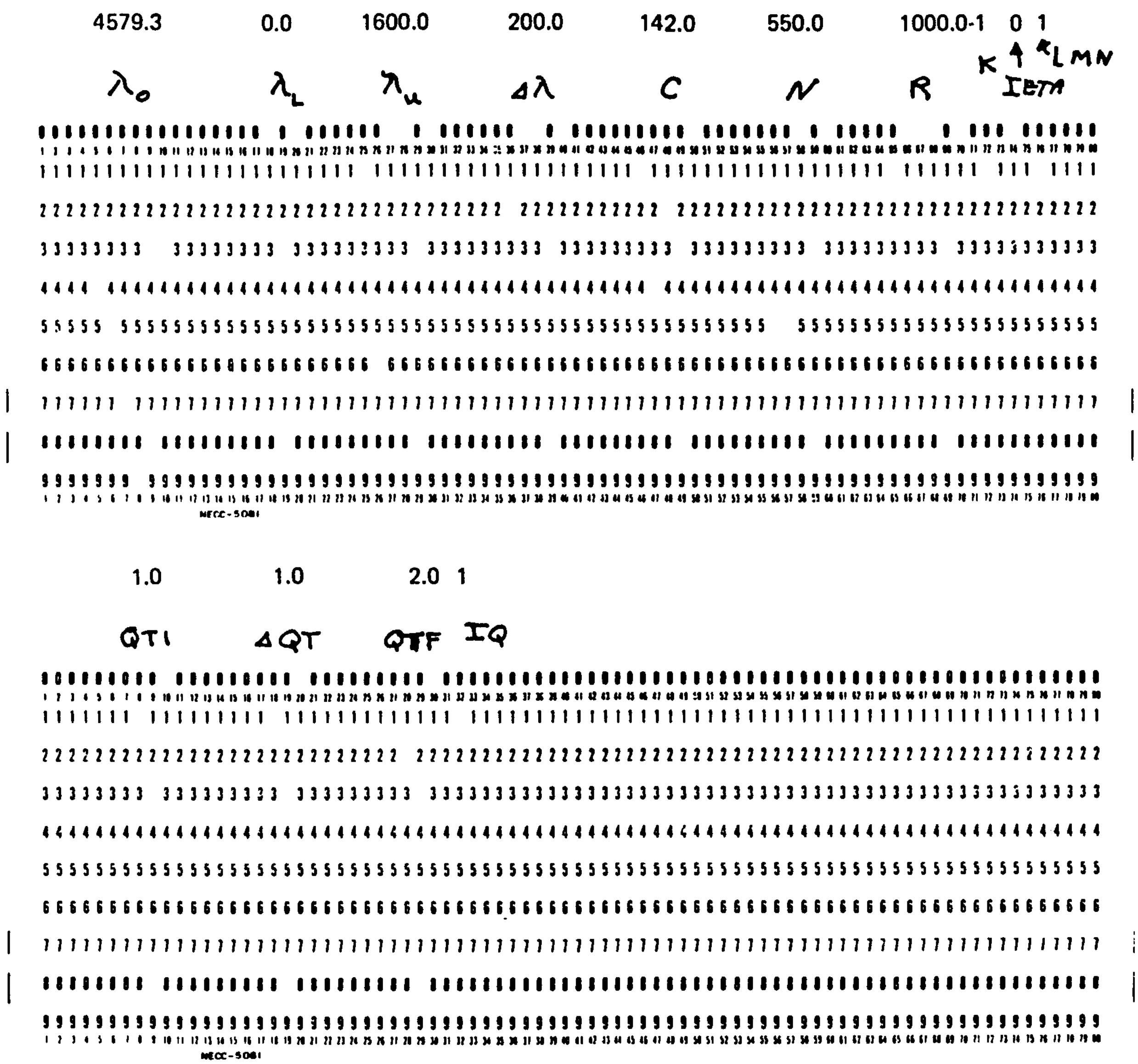

Figure 5. Typical Data Card Set

The first data card is punched using data supplied above and punched in the order listed below:

$\lambda_o = 4579.3$

$\lambda_L = 0.0$

$\lambda_u = 1600.0$

$\Delta\lambda = 100.0$

C = 142.0

N = 550.0

R = 1000.0

K = −1

IETA = 0

LMN = 1

The following is punched on the second data card:

QIT = 1.0

DQT = 1.0

QTF = 2.0

IQ = 1

The output data for the example cited is shown in fig 6 and described as follows:

Line 1 Shows the input parameters; order = −1 is the order of the grating, N = groove frequency in grooves per mm, R = horizontal radius of curvature of the grating in mm. IETA = identifies the design method and LMN = 1 shows that the angle C has been specified.

Line 2 shows the input values for λ_o = LAMDA 0 (Laser Wavelength), λ_L = LAMDA 1 (lower wavelength limit), λ_u = LAMDA 2 (upper wavelength limit).

Line 3 is self-explanatory.

Line 4 shows the calculated instrumental parameters; C = 2K, $\bar{\rho}$ = RHOA, $\bar{\rho}'$ = RHOB, $\bar{r}_o$ = SMLR in mm, and $\bar{r}'_o$ = SMLR in mm. These parameters are defined in the text.

Line 5 shows the values of the torus parameters: Q = q value defined in the text, ρ_t = value of the vertical toroid radius.

Line 7 is self-explanatory and refers to line 8.

Line 8 shows the optimum recording parameters; γ = GAMA, δ = DLTA, ρ_c = RHOC, and ρ_D = RHOD. These parameters are defined in the text.

Line 9 shows the titles for the table showing the performance of the grating as a function of wavelength. The table also shows the comparison of the holographic toroid grating with the toroid conventional grating.

λ = LAMDA is the wavelength at which the grating is evaluated.

$F_{200} \times 10^{-4}$ is the horizontal focus.

F_{020} is the vertical focus and astigmatism.

F_{300} is the first coma term.

F_{120} is the second coma term.

F_{400} is the higher order focusing term.

F_{220} is the toric aberration.

F_{040} is the toric aberration of a higher order

Line 10 shows the holographic grating performance (Modified Method), the value of the wavelength and the values of the aberrations.

Line 11 shows the performance of the conventionally ruled grating (MECH. Ruled).

Line 12 shows that the following information refers to minimizing coma type aberrations for the same instrumental parameters shown in line 4.

Line 13 is self explanatory and refers to line 14.

Line 14 shows the recording parameters γ = GAMA, δ = DLTA, ρ_c = RHOC, and ρ_D = RHOD required to fabricate a toroid grating to minimize coma.

Lines 15, 16, and 17 are defined in the same way as lines 9, 10, and 11 above. The values in this table refer to a grating designed to minimize coma.

*

***** INPUT DATA *****

1 ORDER=-1 N= 550 GROOVES/MM RADIUS= 1000.0 MM IETA= 0 LMN= 1

2 LAMDA0= 4573.3 ANGST LAMDA1= 0.0 ANGST LAMDA2= 1600.0 ANGST

3 *****THE INSTRUMENTAL PARAMETERS*****

4 C= 142.0000 DEG RHOA=0.256472130 01 RHOB=0.372878420 01 SNLR=0.339905910 03 MM SNFRP=0.258162730 03 MM

5 TORUS PARAMETERS: Q=0.965510870 01 TORUS RADIUS=0.103144800 03

6 ASTG TYPE ABERRATIONS MINIMISED......

7 *****RECORDING PARAMETERS******

8 GAMA=-.918423520 01 DLTA=0.626677630 01 RHOC=0.605461240 00 RHOD=0.604545440 00

9

	LAMDA (ANGST)	F200 XE-04	F020	F300	F120	F400	F220	F040
10 MOD. METHOD	0.0	0.159429D 02	-.193178D-01	-.375883D 00	-.345287D 01	0.215530D 01	0.702100D 01	-.393533D 01
11 MECH. RULED		0.159429D 02	-.193178D-01	-.375883D 00	-.345287D 01	0.215530D 01	0.702100D 01	-.393533D 01
MOD. METHOD	200.0	0.534282D 02	-.262283D-01	-.274133D 00	-.443863D 01	0.138237D 01	0.535691D 01	-.531956D 01
MECH. RULED		0.534571D 02	-.184169D-01	-.271496D 00	-.437867D 01	0.138396D 01	0.539664D 01	-.513335D 01
MOD. METHOD	400.0	-.223025D 02	[illegible]	-.175290D 00	-.542567D 01	0.655139D 00	0.115641D 02	-.693833D 01
MECH. RULED		-.222445D 02	[illegible]	-.170010D 00	-.530575D 01	0.658319D 00	0.115636D 02	-.646592D 01
MOD. METHOD	600.0	-.676569D 02	[illegible]	-.797563D-01	-.641332D 01	0.982368D-01	0.147175D 02	-.845245D 01
MECH. RULED		-.675705D 02	[illegible]	-.718403D-01	-.623343D 01	0.103177D 00	0.147167D 02	-.793383D 01
MOD. METHOD	800.0	-.825268D 02	[illegible]	0.120335D-01	-.740085D 01	-.103600D 00	0.176515D 02	-.102826D 02
MECH. RULED		-.824115D 02	[illegible]	0.225954D-01	-.716101D 01	-.397240D 00	0.176574D 02	-.955778D 01
MOD. METHOD	1000.0	-.668020D 02	[illegible]	0.996381D-01	-.938756D 01	-.975530D 00	0.207691D 02	-.122354D 02
MECH. RULED		-.666579D 02	[illegible]	0.112833D 00	-.838776D 01	-.759858D 00	0.217588D 02	-.112783D 02
MOD. METHOD	1200.0	-.203700D 02	[illegible]	0.162790D 00	-.937275D 01	-.112562D 01	0.240368D 02	-.142732D 02
MECH. RULED		-.201570D 02	[illegible]	0.193632D 00	-.901298D 01	-.109790D 01	0.240352D 02	-.131500D 02
MOD. METHOD	1400.0	0.568841D 02	[illegible]	0.260930D 00	-.103557D 02	-.130235D 01	0.274747D 02	-.164746D 02
MECH. RULED		0.570859D 02	-.245777D-01	0.279423D 00	-.993596D 01	-.128922D 01	0.274729D 02	-.151711D 02
MOD. METHOD	1500.0	0.165078D 03	[illegible]	0.333753D 00	-.113356D 02	-.139455D 01	0.317662D 02	-.198136D 02
MECH. RULED		0.165308D 03	[illegible]	0.354873D 00	-.108559D 02	-.137104D 01	0.310640D 02	-.173239D 02

12 .COMA TYPE ABERRATIONS MINIMISED......

13 *****RECORDING PARAMETERS******

14 GAMA=-.616179230 02 DLTA=-.475151560 02 RHOC=0.630857940 01 RHOD=0.145480380 01

15

	LAMDA (ANGST)	F200 XE-04	F020	F300	F120	F400	F220	F040
16 MOD. METHOD	0.0	0.159429D 02	-.193178D-01	-.375883D 00	-.345287D 01	0.215530D 01	0.702100D 01	-.393533D 01
17 MECH. RULED		0.159429D 03	-.193178D-01	-.375883D 00	-.345287D 01	0.215530D 01	0.702100D 01	-.393533D 01
MOD. METHOD	200.0	0.534282D 02	[illegible]	-.274133D 00	-.290535D 01	0.102530D 01	-.822092D 01	-.411841D 02
MECH. RULED		0.534571D 02	[illegible]	-.271496D 00	-.437867D 01	0.138396D 01	0.539664D 01	-.513335D 01
MOD METHOD	400.0	-.223025D 02	[illegible]	-.175290D 00	-.215932D 01	-.195155D-01	-.222916D 02	-.785574D 02
MECH. RULED		-.222445D 02	[illegible]	-.170010D 00	-.530575D 01	0.698319D 00	0.115536D 02	-.646592D 01
MOD. METHOD	600.0	-.676569D 02	[illegible]	-.797563D-01	-.151375D 01	-.973544D 00	[illegible]	-.116986D 03
MECH. RULED		-.675705D 02	[illegible]	-.718403D-01	-.623343D 01	0.103107D 00	0.147167D 02	-.793383D 01
MOD. METHOD	800.0	-.825268D 02	[illegible]	0.120354D-01	-.968138D 00	-.183291D 01	-.528598D 02	-.153741D 03
MECH. RULED		-.824115D 02	[illegible]	0.225954D-01	-.716101D 01	-.397245D 00	0.176504D 02	-.953778D 01
MOD. METHOD	1000.0	-.668020D 02	[illegible]	0.996834D-01	-.221674D 00	-.259316D 01	-.673759D 02	-.191532D 03
MECH. RULED		-.666579D 02	[illegible]	0.112833D 00	-.308276D 01	-.759359D 00	0.217588D 02	-.112783D 02
MOD METHOD	1200.0	-.203700D 02	[illegible]	0.132792D 00	0.426320D 00	-.325058D 01	-.817301D 02	-.229460D 03
MECH. RULED		-.201570D 02	[illegible]	0.198632D 00	-.901299D 01	-.109790D 01	0.240352D 02	-.131500D 02
MOD. METHOD	1400.0	0.568841D 02	[illegible]	0.250985D 00	0.107657D 01	-.390164D-01	[illegible]	-.267526D 03
MECH. RULED		0.570859D 02	-.245777D-01	0.279423D 00	-.993596D 01	-.128922D 01	0.274728D 02	-.151711D 02
MOD. METHOD	1620.0	0.165078D 03	[illegible]	0.333753D 00	0.172979D 01	-.424317D 01	-.109956D 03	-.325730D 03
MECH. RULED		0.165308D 03	[illegible]	0.334873D 00	-.108559D 02	-.137184D 01	0.317640D 02	-.173239D 02

Figure 6.

References:

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