Title
Varied Line-Space Gratings and Applications (invited)

Author
McKinney, W.R.

Publication Date
1991-07-01

LBL-30456

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

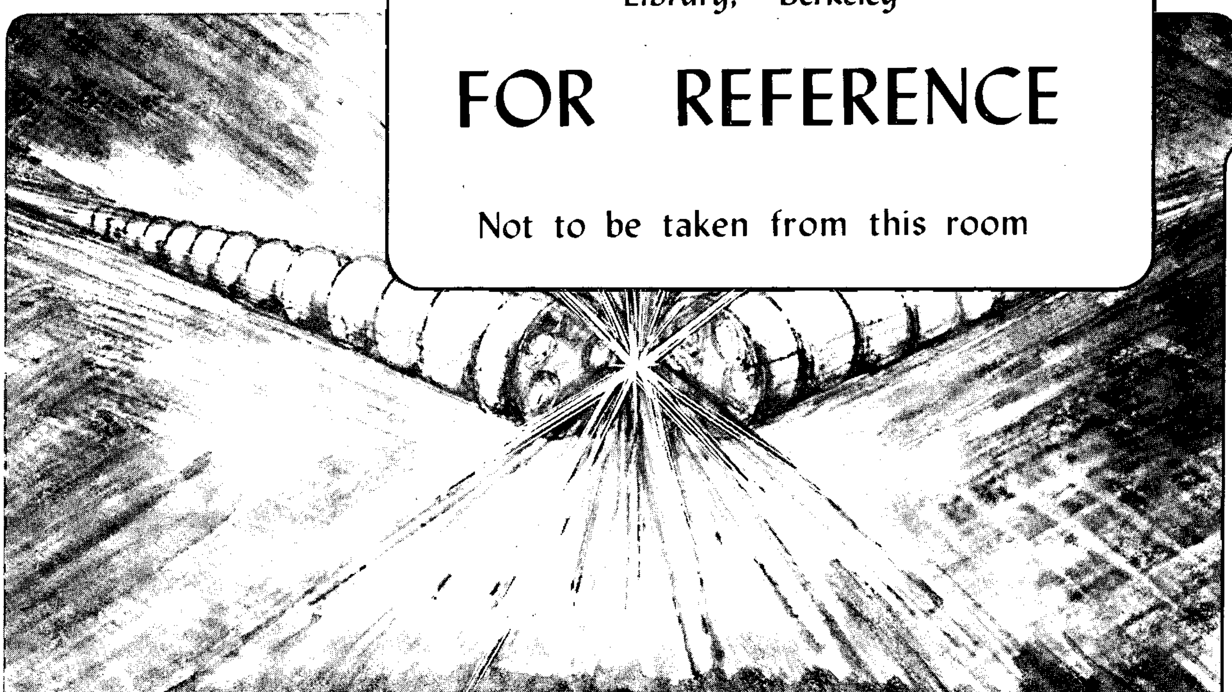
Accelerator & Fusion Research Division

Presented at the Fourth International Conference on Synchrotron Radiation Instrumentation, Chester, UK, July 15–19, 1991,
and to be published in the Proceedings

Varied Line-Space Gratings and Applications

W.R. McKinney

July 1991



Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

DISCLAIMER

DISCLAIMER

LBL-30456

VARIED LINE-SPACE GRATINGS AND APPLICATIONS*

W. R. McKinney

Advanced Light Source
Accelerator and Fusion Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

July 15, 1991

Paper Presented at the 4th International Conference on Synchrotron Radiation Instrumentation,
Chester, United Kingdom, July 15–19, 1991

***This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098**

Varied Line-Space Gratings and Applications*

Wayne R. McKinney

Accelerator and Fusion Research Division
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720 USA

This paper presents a straightforward analytical and numerical method for the design of a specific type of varied line-space grating system. The mathematical development will assume plane or nearly-plane spherical gratings which are illuminated by convergent light, which covers many interesting cases for synchrotron radiation. The gratings discussed will have straight grooves whose spacing varies across the principal plane of the grating. Focal relationships and formulae for the optimal grating-pole-to-exit-slit distance and grating radius previously presented by other authors will be derived with a symbolic algebra system. It is intended to provide the optical designer with the tools necessary to design such a system properly. Finally, some possible advantages and disadvantages for application to synchrotron radiation beamlines will be discussed.

***This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098**

Introduction

Varied line-space (VLS) gratings are of interest to builders of synchrotron radiation instrumentation because these gratings offer an extra degree of freedom to the monochromator designer. This paper will explain enough basic analytical results so that the designer can begin to consider VLS gratings for beamline systems. Although other authors have investigated VLS gratings,[1][2][3][4][5] the contribution of Hettrick and Underwood[6,7] will be emphasized, and the main results in their patent are derived here. Their work, theoretical and experimental, demonstrates the advantages of using VLS gratings with convergent light. However, to our knowledge, their theoretical results have not been previously derived independently or confirmed in the literature.

I. Conventions

Figure 1 shows our coordinate system and the location of the straight and parallel grating grooves. If the blank is curved, the grooves are assumed to be formed by the intersection of the blank and a set of parallel planes. This is just like a Rowland grating, except the distances between the planes may vary. We use the grating equation based on signed angles measured from the normal, which requires the plus sign on the right hand side:

$$m\lambda = \sin(\alpha) + \sin(\beta) \qquad (1)$$

In addition, we assume that all gratings will be used in the standard fixed deviation mounting where the grating is rotated about its center (or pole). (Theta is defined as the incidence angle at zero order, and $2\theta = \alpha - \beta$)

II. Formal Analysis

Hettrick and Underwood pointed out the significant advantage of separating the focusing and dispersing functions for VLS systems. Allowing the focusing element(s) to stay fixed and not rotate provides a system which is much easier to keep in focus as the grating rotates. Figure 2 shows the geometry of the incident wave as it converges onto the grating. We will assume that other optics have created converging wavefronts that have no aberration in the dispersion direction. This would not generally be true in a real application of VLS gratings, but is the natural starting point for the analysis. More detailed analyses that are in preparation show that the focal relationships and VLS spacings that we confirm here give excellent performance.[8] Point A from Figure 1 is now behind the grating, and the virtual object distance OA is negative in the formalism. We write the typical generalized optical path function difference, where $+Nm\lambda$ is added to the geometric path difference to allow for the fact that the diffracted wave is made up of pieces from different incoming wavefronts:

$$F = \langle APB \rangle - \langle AOB \rangle + Nm\lambda \qquad (2)$$

N is the groove number, positive along the +y direction; and, per our convention above, m is positive for the inner order of the fixed deviation mountings that we discuss here. We expand the path function in the aperture variables y and z about the pole of the grating. We have no field variables since we have assumed a perfect converging wave:

$$F = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\left[y\frac{\partial}{\partial y}\right]_{0,0} + \left[z\frac{\partial}{\partial z}\right]_{0,0}\right]^n F \qquad (3)$$

The partial derivatives are applied to the path difference function F in (2). Letting i and j denote the powers of y and z in the coefficients of the series, F_{ij} can be split apart:

$$F_{ij} = M_{ij} + m\lambda N_{ij} \qquad (4)$$

The M_{ij} are the familiar coefficients of Noda, Namioka, and Seya[9] and many other authors. The VLS nature of the grating lies in the N_{ij}:

$$N_{ij} = \frac{1}{n!}\left[\left[y\frac{\partial^{i+j}N}{\partial y^i \partial z^j}\right]_{0,0}\right] \qquad (5)$$

Intuitively, d(y), the local groove spacing, equals:

$$d(y) = \frac{\partial y}{\partial N} \qquad (6)$$

We explicitly are taking d not to be a function of z because of the straight and parallel groove planes. N_{ij} becomes N_i. We now expand d in a manner that will give us VLS coefficients that have a one-to-one correspondence with the familiar aberrations:

$$d(y) = d_0(1 + v_1 y + v_2 y^2 + v_3 y^3 \ldots\ldots.) \qquad (7)$$

Substituting (6) and (7) into (5) gives:

$$N_i = \frac{1}{i!}\frac{\partial^{i-1}}{\partial y^{i-1}}\left[\frac{1}{d_0(1+v_1y+v_2y^2+v_3y^3)}\right]_{0,0} \qquad (8)$$

Using the computer algebraic capabilities of Mathematica™ [Version 1.2 on a Macintosh IIx with 5 MB RAM and a remote kernel operating on a SUN 4 workstation,] the following results were obtained, where the N_i have been substituted into (4):

$$F_{20}\ (\text{defocus}) = M_{20} - \frac{v_1 m\lambda}{2\, d_0} \qquad (9)$$

$$F_{30}\ (\text{coma}) = M_{30} + \frac{1}{6}\left(2v_1^2 - 2v_2\right)\frac{m\lambda}{d_0} \qquad (10)$$

$$F_{40}\ (\text{spherical aberration}) = M_{40} - \frac{1}{24}\left(6v_1^3 - 12v_1v_2 + 6v_3\right)\frac{m\lambda}{d_0} \qquad (11)$$

Since we will be using (9) extensively, we expand it completely, using the expanded sag of the grating surface:

$$x = \sum_{n=0}^{\infty} a_{ij}\, y^i z^j \qquad (12)$$

The a_{ij} are tabulated in Howells.[10] $a_{20} = 0$ for a plane grating, and $a_{20} = 1/(2R)$ for a spherical grating, where R is the radius of curvature.

$$F_{20} = \frac{1}{2}\left[\frac{\cos^2(\alpha)}{r_h} + \frac{\cos^2(\beta)}{r_{hp}} - 2a_{20}\left(\cos(\alpha) + \cos(\beta)\right)\right] - \frac{v_1 m\lambda}{2\, d_0} \qquad (13)$$

This is the paraxial tangential focal condition for a VLS grating.

III. Focal Conditions

We will derive three different focal conditions which give the ratio of the optimal real distance to the focal plane as a function of the assumed virtual focal distance behind the grating and the angles of incidence and diffraction at the chosen wavelengths of optimization. Each succeeding focal condition will be better than the previous in focusing correction, but it should be emphasized that the VLS focusing correction for convergent incident light is so powerful, that the simpler ones can form the basis of excellent monochromator designs.

In exact analogy to the design of other constant deviation monochromators[11] with fixed entrance and exit distances onto the grating (r_h and r_{hp}), we set the defocus aberration equal to zero at two wavelengths in the region of interest:

$$[F_{20}]_{\lambda=\lambda_1} = [F_{20}]_{\lambda=\lambda_2} = 0 \qquad (14)$$

Considering r_h and r_{hp} the independent variables, some manipulation that does not need the computer gives the equivalent to Equation #3 of Hettrick and Underwood's patent.[12] They use a different form of the grating equation, and define r_h as positive. The incidence and diffraction angles (α s and β s) are determined by the fixed deviation geometry:

$$\frac{-r_{hp}}{r_h} = \frac{\lambda_1\cos^2\beta_2 - \lambda_2\cos^2\beta_1}{\lambda_1\cos^2\alpha_2 - \lambda_2\cos^2\alpha_1} \qquad (15)$$

Even though v_1 has disappeared, it can be found using either of the equations in (14). We now choose a parameter set that will allow us to compare this focal condition with later ones. It is shown in table 1, and is the same set used in McKinney and Palmer.[13] We obtain r_{hp}/r_h = -1.0044775, and v_1 = 1.986225/meter. If we assume a large plane (a_{20} = 0) grating of 20 cm width, the variation in groove spacing is only +/- 20%, which is reasonable to fabricate on a ruling engine. Of particular significance is the fact that r_{hp}/r_h is very close to 1. Since the straight and parallel grooves give no sagittal power, it is very important that the natural r_{hp} of best tangential focus is very near the sagittal focus of the converging wave, because it gives an approximately stigmatic image. Thus, this type of grating system gives good imaging behavior as a natural consequence of the design. As a confirmation of the value Hettrick and Underwood's contribution, we check the focusing for non-converging (parallel) incoming light onto a plane VLS grating. (r_{hp}-> -infinity) Only the second and fifth terms of equation (13) remain, and we have only r_{hp} as a parameter:

$$r_{hp} = \frac{d_0}{v_1}\frac{\cos^2\beta}{m\lambda} \qquad (16)$$

We can only focus the grating at one wavelength, and v_1 is just a scaling factor like the power of a lens or zone plate. Varying it moves a focal curve of fixed shape either toward or away from the grating, and does not change the shape of the curve as it does when converging light is used.[13]

To achieve Hettrick and Underwood's second focal condition , we set:

$$[F_{20}]_{\lambda=\lambda_1} = \left[\frac{\partial F_{20}}{\partial\phi}\right]_{\lambda=\lambda_1} = 0 \qquad (17)$$

where phi indicates differentiation with respect to the scan angle of the grating, and λ_1=30 Angstroms. To do this we change variables:

$$\phi = (\alpha+\beta)/2 \quad \theta = (\alpha-\beta)/2 \qquad (18)$$

The scan angle is signed the same as alpha and beta, and the half deviation angle (87 degrees for our test case) is positive definite. After taking the derivative, we eliminate v_1 from equations (17) and solve them for r_{hp}/r_h:

$$\frac{r_{hp}}{r_h} = \frac{-\cos\beta_1(\cos\alpha_1\cos\beta_1 + \cos^2\beta_1 + 2\sin\alpha_1\sin\beta_1 + 2\sin^2\beta_1)}{\cos\alpha_1(\cos\alpha_1\cos\beta_1 + \cos^2\alpha_1 + 2\sin\alpha_1\sin\beta_1 + 2\sin^2\alpha_1)} \qquad (19)$$

With the same reminders about sign conventions, we recognize equation #4 from the Hettrick and Underwood's patent. Using our test case we see that r_{hp}/r_h = -1.00546, and v_1 = 1.98475/meter. Note that the both the linear VLS coefficient and the optimal focal distance have not changed significantly, and our previous conclusions are still valid.

For our third and most complicated focal condition, we set:

$$[F_{20}]_{\lambda=\lambda_1} = [F_{20}]_{\lambda=\lambda_2} = \left[\frac{\partial F_{20}}{\partial \phi}\right]_{\lambda=\lambda_1} = 0 \qquad (20)$$

This is a combination of both of the first two cases, (λ_1=20 Angstroms, and λ_2=40 Angstroms) and requires another degree of freedom. Following Hettrick and Underwood, we choose to modify the plane grating with a long radius of curvature, and hope that we can do it without spoiling the basic premise of separation of focusing and dispersion. We change a_{20} to 1/(2R), which results in a focal curve equation with 5 terms (13). Eliminating v1 and R from the three equations (20), and then solving for r_{hp}/r_h gives:

rhp/rh=numerator/denominator (21)

numerator=

**-((cosα1*cosα2*cosβ1^2+cosα2*cosβ1^3+cosα1*cosβ1^2*cosβ2
+cosβ1^3*cosβ2-cosα1^2*cosβ2^2-2*cosα1*cosβ1*cosβ2^2-
cosβ1^2*cosβ2^2-cosβ2^2*sinα1^2+cosβ1^2*sinα1*sinα2+
2*cosα2*cosβ1*sinα1*sinβ1+2*cosβ1*cosβ2*sinα1*sinβ1-
2*cosβ2^2*sinα1*sinβ1-
2*cosα1*cosβ1*sinα2*sinβ1-cosβ1^2*sinα2*sinβ1+
2*cosα2*cosβ1*sinβ1^2+
2*cosβ1*cosβ2*sinβ1^2-cosβ2^2*sinβ1^2+cosβ1^2*sinα1*sinb2-
2*cosα1*cosβ1*sinb1*sinβ2 - cosb1^2*sinβ1*sinβ2)**

denominator=

**(cosα1^3*cosα2-cosα1^2*cosα2^2+cosα1^2*cosα2*cosβ1-
2*cosα1*cosα2^2*cosβ1-
cosα2^2*cosβ1^2+cosα1^3*cosβ2+cosα1^2*cosβ1*cosβ2+
2*cosα1*cosα2*sinα1^2-
cosα2^2*sinα1^2 + 2*cosα1*cosβ2*sinα1^2-cosα1^2*sinα1*sinα2-
2*cosα1*cosβ1*sinα1*sinα2+2*cosα1*cosα2*sinα1*sinβ1-
2*cosα2^2*sinα1*sinβ1 +
2*cosα1*cosβ2*sinα1*sinβ1+cosα1^2*sinα2*sinβ1- cosα2^2*sinβ1^2 -
cosα1^2*sinα1*sinβ2 -
2*cosα1*cosβ1*sinα1*sinβ2 + cosα1^2*sinβ1*sinβ2))**

Any of the equations (20) may be solved for the radius of the grating and we can now recognize that this result is not the same as to equation #5 of Hettrick and Underwood's patent. Our test case provides r_{hp}/r_h = -0.99041, and v_1 = 2.00957/meter, and R = +4364.05 meters (+ is concave), confirming our belief that the curvature of the almost plane grating would be only a small perturbation, and that the focal condition and variation in the line spacing would be similar in magnitude to those of the earlier conditions. Hettrick and Underwood's equation #5, which is apparently incorrect, gives values which do not conform to these assumptions.

III. Summary of Analytical Results

Figure 3 shows F_{20} as a function of wavelength for the three focal conditions derived above. We see that our focal curves satisfy the conditions of derivation. Curve 1 goes through zero twice at 20 and 40 Angstroms, satisfying the first of our focal equations. Curve 2 goes through zero only once, at 30 Angstroms, and has zero derivative there, consistent with the assumptions the derivation of our second focal curve. The higher order curve 3 satisfies all three of the conditions (20) which are permitted by allowing the grating to have a small degree of curvature. To our knowledge this type of VLS monochromator has not yet been constructed.

IV. Higher Order VLS Corrections

Hettrick and Underwood's equation #6 is their analog of our expression for the groove spacing (7). Their ε_1, ε_2 and ε_3 are numerically not the same as our v_1, v_2 and v_3, since they expand the groove function differently. Our analogs of their equations #7 are simply found by using one of the three above conditions for obtaining v_1. r_h takes an assumed value. Then the one of our equations (15) (19) or (21) gives r_{hp}. To obtain v_2, the parabolic VLS coefficient related to coma, we pick any wavelength in the range, (Hettrick and Underwood choose $(\lambda_1+\lambda_2)/2$) and solve (10) for v_2 using the previous r_h, r_{hp} and v_1. For v_3, the cubic VLS coefficient related to spherical aberration, we solve (11) for v_3 using the previous r_h, r_{hp} and v_1 and v_2.

V. Summary and Conclusions

We now have outlined an analytical, scale independent method for designing a plane or slightly spherical VLS constant deviation monochromator with light converging behind the grating. Even though we find equation #5 of Hettrick and Underwood's patent to be in error, the bulk of their analysis is correct, and their emphasis of separating the focusing and dispersing functions for VLS systems is shown to be a very useful contribution to monochromator design.

The VLS design, as described here, has several advantages.

1. The corrected focal curve eliminates the need for moving slits, which are required to keep a Rowland Circle monochromator in focus.
2. The separation of focusing and dispersion allows a plane grating to be used, which is less expensive to manufacture. Even though our third and best focused condition requires a slight curvature to the grating, the plane grating conditions give excellent focal correction, and therefore excellent performance.[14]
3. Although we have not demonstrated it explicitly, since we only consider elementary second order focusing, the extra degree of freedom to move the groove placement should provide higher angular acceptance at a given resolving power than any other design.

4. The VLS coefficients provide the opportunity to reduce some of the aberrations of the converging optics. (This is discussed in the patent of Hettrick and Underwood.[12]

The VLS system also has some disadvantages:

1. Since holographically generated VLS gratings are not commercially available ruled gratings must be used which would likely have more stray light. It has been shown that holographic gratings can be made equivalent to VLS gratings,[15] and in the future this may be exploited allowing wider use of VLS systems.
2. The separation of dispersion and focusing requires at least two optics between the slits which increases cost and the possibility that surface imperfections may affect imaging.
3. The ruling engine may not have the capability to adjust the shape of the groove as the grating is ruled, resulting in less that optimal efficiency all across the grating.

4. Finally the VLS monochromator shares several undesirable features of the standard type spherical grating monochromator.[16 17 18] The fixed deviation design that is common to both requires multiple gratings for an extended wavelength range on account of the horizon wavelength condition. In addition, the VLS grating is not used in the on blaze condition at all wavelengths. Worse still, the fixed deviation geometry of both leads to serious higher order problems at longer wavelengths.

The VLS monochromator does not solve all of the problems of designers of grating-based monochromators for VUV beamlines. VLS gratings do provide advantages that should be considered when choosing a monochromator configuration. We believe that VLS gratings will have an increasing role at synchrotron radiation sources in the future. We have compared the analytical methods presented here with numerical optimizations, and find that the analytical formulae give designs which for practical purposes are sufficiently close to the numerically optimized ones.

Acknowledgement

The author wishes to acknowledge his extensive collaboration on monochromator design in general, and VLS systems in particular with Christopher Palmer, and to thank both he and Malcolm Howells for critically reading the manuscript.

---

[1] Y. Sakayanagi, Science of Light **16**, No. 2, 129 (1967)

[2] T. Harada and T. Kita, Applied Optics **19**, 3987 (1980)4)

[3] T. Harada, M. Itou, and T Kita, Proc. SPIE **503**, 114 (198

[4] Murty, M., J. Opt. Soc. Am. **57**, 768 (1962)

[5] M. Pouey, Nuclear Instruments in Physics Research, A 246, 256 (1986)

[6] M.Hettrick, Applied Optics **24**, 1737 (1985)

[7] M.Hettrick, and J. H. Underwood, AIP Conf. Proc. **147**, 237 (1986)

[8] McKinney and Palmer, manuscript in preparation.

[9] H Noda, T.Namioka and M. Seya J. Opt. Soc. Am. **64**, 1031 (1974)

[10] Howells, M. R., Brookhaven National Laboratory Informal Report 27416 (1980)

[11] W. McKinney and M. R. Howells, Nuclear Instruments and Methods, **172**, 149 (1980)

[12] M. Hettrick, and J. H. Underwood, U. S. Patent #4776696 (1988)

[13] W. R. McKinney and C. Palmer, Proc. SPIE **1055**, 332 (1989)

[14] M. Hettrick, J. H. Underwood, P. Batson, and M. J. Ekhart, Applied Optics **27**, 200 (1988)

[15] C. Palmer and W. R. McKinney, Applied Optics **29**, 47 (1990)

[16] W. R. McKinney, M.R. Howells, T. Lauritzen, J. Chin, R. DiGennaro, E, Fong, W. Gath,J. Guigli, H Hogrefe, J. Meneghetti, D. Plate, P. A. Heimann, L. Terminello, Z. Ji, D. Shirley, and F. Senf, Nuclear Instruments and Methods in Physics Research, A291, 221 (1990)

[17] H. A. Padmore, Rev. Sci. Inst. **60**, 1608 (1989)

[18] C T, Chen and R. Sette, Rev. Sci. Inst. **60**, 1616 (1989)

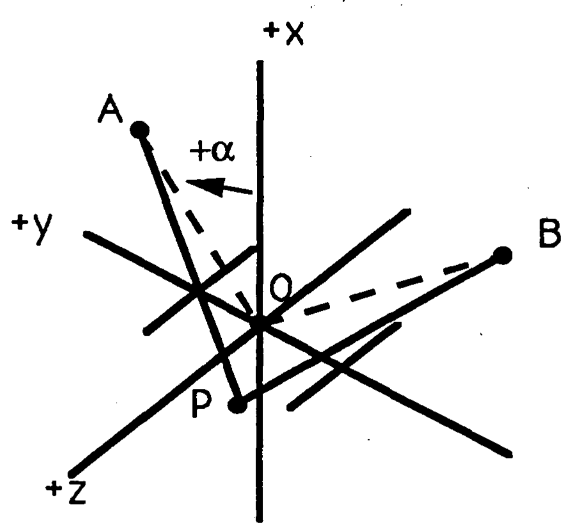


Fig. 1. Coordinate System and location of the grooves and the image and object points.

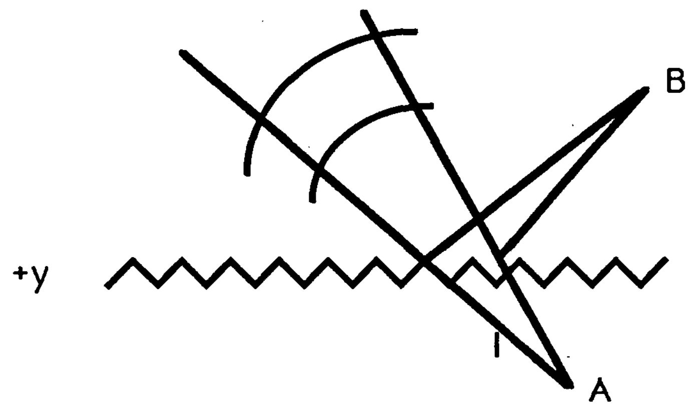


Fig. 2. Geometry of wavefronts onto VLS grating.

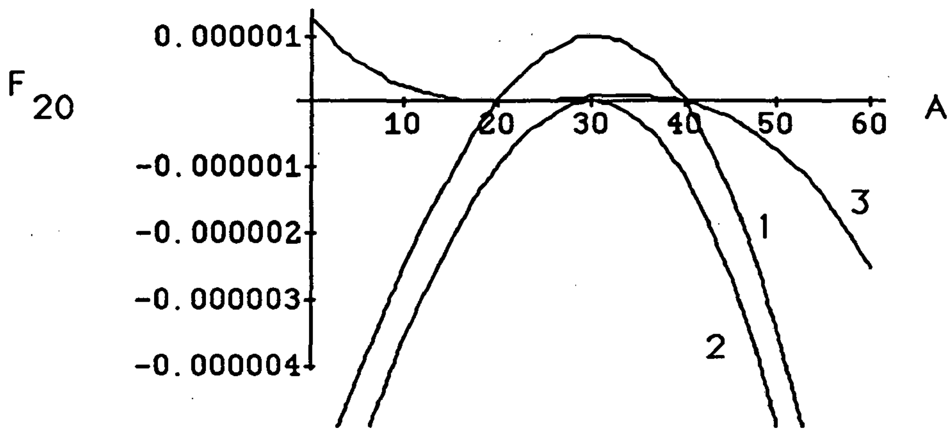


Fig. 3. The defocus aberration as a function of wavelength for the three different focal conditions.

Table 1. Monochromator Parameters for Comparison Case

half deviation angle	=	87 degrees
order of diffraction	=	+1 (inner order: $\lvert\beta\rvert < \alpha$)
wavelength range	=	20 Angstroms to 40 Angstroms
incident light converging 1 meter behind the grating		
grooves per mm	=	1200 at the center of the grating