Light Source Note: LSBL- 362
Author(s) Initials
Group Leader's initials
Date 2/25/97
Date 3/5/97

SIGN CONVENTIONS IN THE USE OF THE OPTICAL PATH FUNCTION IN GRATING THEORY

M.R. Howells, W. R. McKinney, Advanced Light Source, LBNL
C. Palmer, Milton Roy, Company, Rochester NY.

In using the optical path function development of grating theory it is conventional to calculate the distance F along the path APB where A is the source point, B the arrival point and P a general point on the nth groove of the grating. For wavelength λ one then normally expresses the optical path for a ray diffracted in mth order as

$$F = \langle \mathrm{AP} \rangle + \langle \mathrm{PB} \rangle + nm\lambda \tag{1}$$

The geometry is shown in Fig 1 which is taken from [Noda et al. 1974][2]. Like many other authors Noda et al adopt the convention that the signs of the angles of incidence (α) and diffraction (β) measured from the normal are opposite if the angles are on opposite sides of the normal. If we, in addition, follow usual practice and take λ and the grating spacing d to be positive, this leads to a grating equation

$$m\lambda = d(\sin\alpha + \sin\beta) \tag{2}$$

In order to use equations (1) and (2) consistently we have to make proper choices of the sign of either α or β, the sign of m and the direction of the incoming ray which can be toward $+y$ or toward $-y$.

First suppose that we define α positive and consider a ray diffracted in inside order (meaning that the diffracted ray lies between the inward and zero-order rays). For inside order we must have $|\alpha| > |\beta|$ so that $\sin\alpha + \sin\beta$ must be positive. Therefore m must be positive for this case. Similarly if we had defined α negative, then $\sin\alpha + \sin\beta$ would have been negative so that m would also have needed to be negative. Thus we conclude that for (2) to remain true we must have

For α defined:	**the order convention must be:**
Positive	inside is positive
Negative	inside is negative

Now consider the part of a wavefront being diffracted by a single groove in inside order as shown in Fig.2 and suppose initially that we have chosen the "α–is-positive, inside-order-is-positive" convention. It is clear from the figure that for inside order the distance $d\sin\alpha$ is greater than $d\sin\beta$. This implies that the path via G is longer than via F. Thus for the present case, equation (1) will be true only if n increases by one in passing from F to G. Now the assumption of positive d and the general definition of n by

$$\frac{1}{d(y)} = \frac{\partial n}{\partial y}, \tag{3}$$

implies that n increases toward $+y$. Therefore the above argument shows that in the case at hand, the ray progresses toward +y.

Similarly, if the "α–is-negative, inside-order-is-negative" convention is chosen, the G path is still longer than the F, so n must now diminish by one in passing from F to G. In this case, the assumption of positive d coupled with equation (3) implies that the direction of progress of the ray must now be toward $-y$. In summary, assuming positive d and equation (3) as the definition of n, we have

For the ray direction	**the α and order conventions must be:**
Toward $+y$	α positive, inside is positive
Toward $-y$	α negative, inside is negative

This conclusion has particular importance in making a consistent treatment of holographic and varied-line-spacing (VLS) gratings because the groove pattern along the y axis is then not symmetrical about y=0.

In using the SHADOW ray-trace code it is said that the conventions adopted by the code are that inside-order-is-negative and the ray progresses toward $+y$ (the sign of α is invisible to the user). This is not in agreement with the above assumptions and conventions. However one could adapt to it for ray tracing VLS gratings by altering the grating prescription[1]

$$d(y) = d_0\left(1 + v_1 y + v_2 y^2 + v_3 y^3 + \ldots\right) \tag{4}$$

so that $d(-y) \Rightarrow d(y)$. This can be accomplished by reversing the signs of the odd power coefficients in (4) before (or after) making the appropriate translation to SHADOW notation. Physically it is equivalent to using the same grating but turning it around in the instrument. We are not familiar enough with the code to know if the above conventions are really fixed or whether there is some way the user can choose the convention to avoid the above contortion in entering the VLS data. Franco Cerrina has now responded to our letter on this point and his discussion is attached as Appendix 1.

In the table below we show how some treatments of grating theory which are of particular interest to us deal with the conventions we have been discussing. Such conventions are mostly a matter of choice but certain limitations on the choice have to be respected to maintain consistency. Moreover, some of the choices can be left open while writing down the theory but must be made consistently in order to apply the theory.

Conventions for:	**Noda 1974**	**McKinney 1992**	**Palmer 1994**[3]	**SHADOW**
d or $d(y=0)$	always +	always +	always +	invisible
λ	always +	always +	always +	invisible
α, β signs w.r.t. normal	opp on opp sides	opp on opp sides	opp on opp sides	invisible
α	none	+	sign(α)=sign(y)	invisible
m for inside order	none	+	sign(m)=sign(α)	–
Optical path equation	eq 1	eq 1	eq 1	invisible
Grating equation	eq 2	eq 2	eq 2	invisible
n	eq 3	eq 3	eq 3	invisible
Ray progresses toward	$-y$*	$-y$*	$+y$*	$+y$

*These choices are expressed only in the diagrams and do not change the written form of the theory.

References

1. McKinney, W. R., "Varied line-space gratings and applications", *Rev. Sci. Inst.*, **63**, 1410-1414 (1992).

2. Noda, H., T. Namioka, M. Seya, "Geometrical Theory of the Grating", *J. Opt. Soc. Am.*, **64**, 1031-6 (1974).

3. Palmer, C., W. R. McKinney, "Imaging theory of plane-symmetric varied line-spacing grating systems", *Opt. Eng.*, **33**, 820-829 (1994).

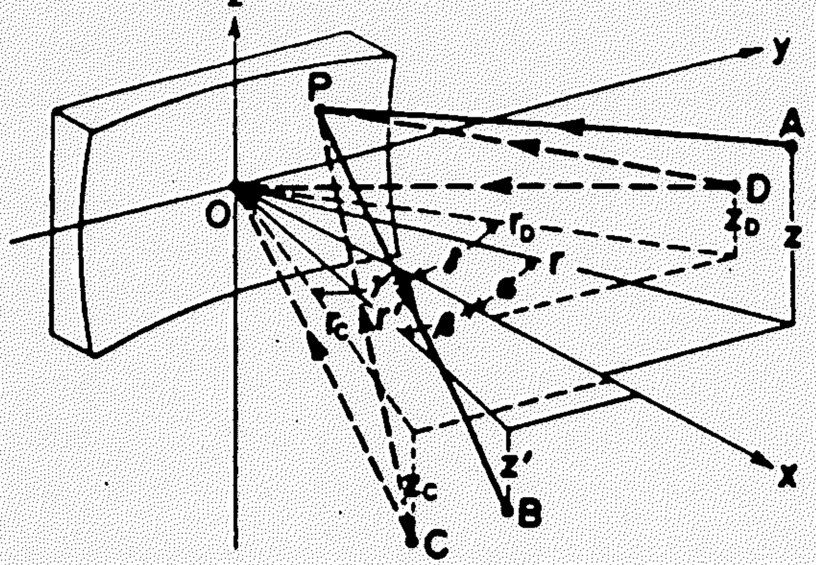
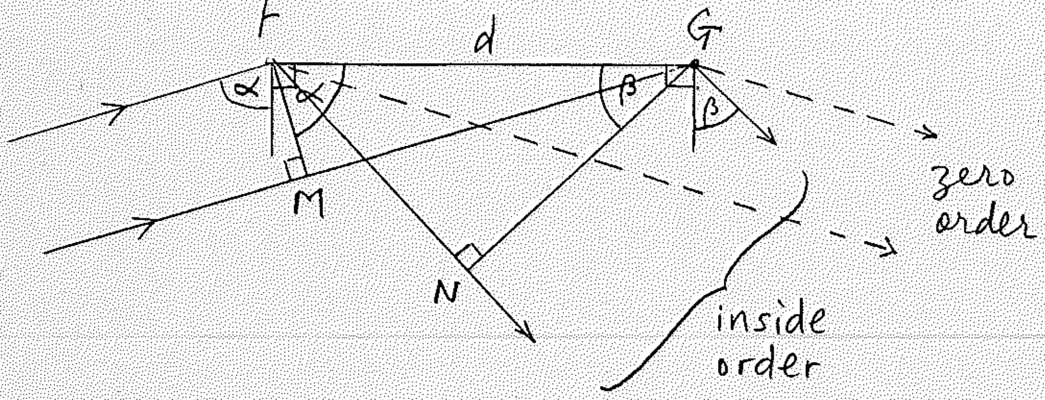


Fig 1



$FN = d \sin\beta$

$GM = d \sin\alpha$

Fig 2

APPENDIX 1

University of Wisconsin
Center for X-ray Lithography

January 9, 1997
F. Cerrina

CAMPUS OFFICE:
1415 Johnson Drive
Madison, WI 53706-1691
(608) 263-4955
Fax (608) 265-3811
cerrina@xraylith.wisc.edu

Dear Malcolm, Chris and Wayne:

I finally got around to answer; I had the letter sitting on my computer for a while, but something else always seemed to have higher priority.

First, I'd like to thank you for finding the time to point out what seems to be a problem in SHADOW. In any case, there seems to be a different philosophy in dealing with diffraction, and hence a different terminology. While you take an approach based on the expansion of the optical path, we take an approach based on diffraction and scattering theory. Let me explain how we treat diffraction, and things should become clear.

Franco

Diffraction

The main point to consider is that we take an approach based on Fourier analysis rather than on the computation of the optical path. [1] In general, if $d(x, y)$ is the local line density (i.e., the surface spatial frequency f_x) on the grating surface, we define a two-dimensional scattering vector $\vec{q_{||}}$ as:

$$\vec{q_{||}} = 2\pi d\ \vec{\tau} \tag{1}$$

where $\vec{\tau}$ is orthogonal to the groove and tangent to the grating surface. Thus the vector $\vec{q_{||}}$ belongs to the plane tangent in (x, y) and is orthogonal to the local groove. The diffraction condition for a ray is computed using the Bragg equation:

$$\vec{k'} = \vec{k} + m\vec{q_{||}} \tag{2}$$

together with the total momentum conservation

$$|\vec{k}| = |\vec{k'}| \tag{3}$$

which is guaranteed by the solid response; m is the index of the surface scattering vector participating in the process. Thus, the diffraction from a surface grating is completely analogous to the treatment of surface diffraction as found, for instance, in LEED. Notice that no hypothesis is made on the relative orientation of $\vec{k}$ and $\vec{\tau}$; conical diffraction is easily computed.

Notice also that $\vec{k}, \vec{k'}$ are expressed in the local reference trihedron, formed by *normal, tangent* and *bi-normal*. Indeed, much of the work goes in keeping track of the correct change of reference frames back and

[1] A good treatment is found, for instance, in the book "Diffraction Physics" by J.M. Cowley, North Holland, 1984

forth between local (trihedron) and global (mirror). These equations predict correctly the diffraction of a ray. In agreement with the scattering point of view, **we define a value of $m = -1$ as an inside order, since the scattering vector will be oriented toward $-x$ direction**. A similar point of view is taken, for instance, in LEED.

In this definition there is no need of tracking the sign of angles, since they are automatically handled by the scattering theory. Furthermore, in SHADOW we attempt to never compute angles explicitely, and we prefer to rely on vector calculus in order to improve accuracy and speed. Unfortunately, this means that it is not possible to easily implement traditional optics definitions of positive and negative angles and distances in object and image space; nor would we want to, because of the great simplicity which is obtained using the vector formulation.

Application to Variable Line Spacing Gratings

These were introduced during a collaboration with Michael Hettrick, and follow the convention he requested. (Another case is that of the so-called "oriental fan".) The coefficients are used to compute the local line density $d(x, y)$, and this is used to compute the scattering vector (see above). Thus SHADOW can compute arbitrary diffraction gratings, as long as the ruling function is known either analitically or as a table (possibly measured experimentally) over the grating surface. Notice that SHADOW follows the figure of the mirror, since $\vec{q}_{||}$ is always computed in the tangent plane.

The formulae used for the computation of the local ruling density refer to a one-dimensional case only, and are quite simple. Essentially, the line density $d(x, y)$ is expressed as a polynomial function of the distance y to the intercept point; i.e., $d(x, y) = d(y)$. Notice that the formula is completely independent of angles, and has no knowledge of the order selected. SHADOW computes the intercept, figures the local trihedron, computes the local line density, aligns the scattering vector orthogonal to the groove and then computes the scattering process using Bragg's formula. The incidence angle is *implicitly* contained in $\vec{k}$, but does not need to be ever computed explicitly in order to solve the diffraction.

This is the listing of the code fragment that computes the local line density:

```
C
C Compute now the adjustment to the surface line density at the point
C of intercept
C
      CALL DOT (VNOR,Y_VRS,G_FAC)
      G_FAC =   SQRT (1.0D0 - G_FAC**2)
C
C Computes distance of intercept projection on basal plane from
C origin.
C
      TTEMP =   PPOUT(3)/VVIN(3)
    DIST =   PPOUT(2) + VVIN(2)*TTEMP
C
C Test for sign flag
C
      IF (F_RUL_ABS.EQ.0) DIST = ABS(DIST)
    RDENS =   RULING + RUL_A1*DIST + RUL_A2*DIST**2
     $ + RUL_A3*DIST**3 + RUL_A4*DIST**4
    G_MODR =   RDENS*TWOPI*ORDER*G_FAC
  END IF
```

The variables `Ruling, Ruling_A1, ...` are the `a_0,a_1,...` coefficients listed in the input session. They are in various powers of cm^{-1} because SHADOW uses cm^{-1} to store the wavevector of each ray. `G_MODR` is the amplitude of $\vec{q_{\|}}$ discussed above, and will be added to $\vec{k}$ a few steps later.

Finally, the cryptic question about the *Absolute* or *Signed* is understood by considering that $d(x,y)$ can be made function only of the absolute distance from the origin, i.e., $|x|$ (absolute), or of just plain x (signed).

Mike had a need for this feature. Notice that the set of variables (x, y) refer to the basal plane, the idea being that the gratings were mechanically ruled.

We have also a very general 2-d feature, whereby `RDENS` is made dependent on a two-dimensional polynomial, but we never released it. It allows, for instance, to easily model reflective Fresnel Zone Plates. Let me know if you are interested, I could dust it off.

Conclusion

SHADOW handles diffraction with a unified treatment that is suitable for diffraction gratings, crystals and roughness. In all these cases the base approach is the same. It is based on Fourier optics, and implemented in term of scattering theory; I believe that this is one of the strengths of SHADOW, i.e., the use of very general models that can be easily extended without altering the code itself.

I hope that this brief discussion clarifies the implementation of the model.

be careful withe the coeff of odd powers