AXAF Transmission Grating Diffraction Coordinates

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1 Overview of AXAF Transmission Grating Spectrometers

AXAF has two transmission grating spectrometers, the High Energy Transmission Grating Spectrometer (HETGS) and the Low Energy Transmission Grating Spectrometer (LETGS). Each operates by placing a toroidal support structure tiled with diffraction grating facets behind the mirror assembly. The photons are collected on a detector approximating another inner portion of the same torus (this is known as a Rowland geometry). The HETG plate actually combines two toroids which are coaxial, but rotated relative to each other so as to act as two spectrographs: the outer two mirror shells illuminate the Medium Energy Grating (MEG) and the inner two form the High Energy Grating (HEG. The HEG and MEG operate simultaneously.) A schematic perspective view of the Rowland torus is shown in Figure 1. (For overviews of HETG and LETG configurations and performance, see the ASC's Science Instrument Notebook.)

URL for the SIN (Science Instrument Notebook): http://hea-www.harvard.edu/asc/SIN/SIN.html

Each grating (HEG, MEG, or LEG) disperses photons into a plane (approximately) which forms a line (approximately) when sampled by a detector. Optical aberrations and scattering will distort the line somewhat, but there is a plane of symmetry defined by the mid-plane of the torus. (The symmetry may be broken between the positive and negative order sides due to grating efficiency effects. Grating efficiency models are described elsewhere.)

For grating efficiency models, see Markert, Davis, and Dewey, 1995, SPIE, 2518, 424 (HETG), or Lochbihler, Predehl, and Tesche, 1994, Optik, No. 2, p. 1 (LETG).

Ray-trace models describe the physical interactions of photons with each optical element and project rays from one element to the next. From the observational point of view, however, there is practically no knowledge of the photon direction from the support structure (i.e., which facet) to the detecting pixel. Observationally, the photons are treated as if they originate from an average grating placed at the grating *node* — a fictitious point representing the intersection of the optical axis with the Rowland torus, and nominally near the physical center of the grating support structure.

Some information on photon direction can theoretically be obtained from aberrations such as astigmatism; more could be gotten from a de-focused image.

The quantity of interest to be determined from the observed photon is the diffraction angle in the plane of diffraction that the photon makes with the

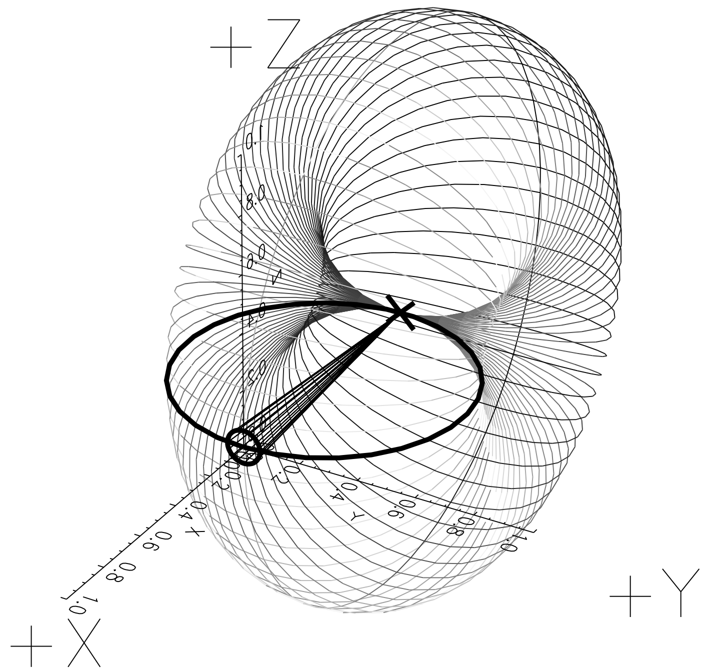

Figure 1: *This figure shows a perspective mesh view of a torus. The axes represent an AXAF coordinate system, with the origin at the grating node, $+x$ coming mostly towards the viewer and the mirror assembly, $+y$ going towards the right and roughly showing the dispersion direction, and $+z$ going up, being the instrument translation direction. The gratings would form a small toroidal cap at the origin (a scaled circle is barely visible), and the $\times$ marks the focal point. The Rowland diameter has been scaled to unity. The dark circle in the $x-y$-plane through the origin is the on-axis Rowland circle. A cone of rays is drawn converging from the grating to the detector.*

direct-beam direction. That angle is very nearly linearly proportional to the photon wavelength with a high constant of proportionality (i.e., high resolution).

It is the purpose of this document to define the inverse transformation of detected photon position to diffraction angle in a *grating nodal coordinate system.*

2 Grating Nodal Diffraction Coordinates

The direct beam of un-diffracted photons, also known as the zero-order, will produce an image of the source on the detector. The location of this image serves as a reference point for the diffracted photons. The dispersion direction is defined by the direction perpendicular to both the nodal axis (the line between the grating node and the source image position) and the average grating bar direction. This is a reference direction, of which there are three, one for each of the HEG, MEG, and LEG gratings. Two more important directions are the direction from the grating node to the source image, and from the node to a photon whose grating nodal coordinates are to be determined.

A diagram (Figure 2) will help clarify the important parameters and define quantities for the transformation.

2.1 Definitions

Refer to Figure 2 for a view of the geometry.

Notation: Vectors will be shown with an arrow, as $\vec{S}$, and represent a position vector from the origin. A single component of the vector will be represented with a subscript, as S_x. A coordinate in three dimensions will be denoted by S without the arrow, and represents the triplet, (S_x, S_y, S_z). Unit vectors (the norm) will be denoted by a *hat*, as in $\hat{r}$. The magnitude of a vector is denoted as in $|\vec{S}|$. A line segment is denoted by a concatenation of points, as in NS, and an angle by concatenation of three points, as in NSD. Cartesian coordinate systems are right-handed; rotations are also right-handed.

A right had rule means point the fingers of your right hand toward $+x$; they then curl toward $+y$ and the thumb points to $+z$. For angles, point your right thumb in a direction; the fingers curl in the direction of positive angle.

N Grating Node; diffracted photons appear to originate from the grating node. The node is nominally on the HRMA x-axis. This is defined as the origin for diffracted photons, namely the point $N = (N_x, N_y, N_z) = (0, 0, 0)$. We imagine an average grating facet is located here.

B Boresight, also referred to as the aim-point. This is nominally at best focus (but detector could be off-nominal focus) and nominal origin of (y, z) plane. The source will typically be very near B, but in general could be off-axis.

While $y - z$ define a plane, the detectors in general don't. The spectroscopic detectors tile the Rowland circle — they come out of the plane in the $+x$ direction.

S Source centroid; centroid of zero-order image. The source is nominally at B, but could be at some arbitrary off-axis angle. In fact, due to dither, it is guaranteed to be off-boresight. It is not necessarily in the $y - z$ plane.

D Diffracted photon event location. This is also not necessarily in the $y - z$ plane.

α Clocking angle of dispersion direction relative to the y-axis.

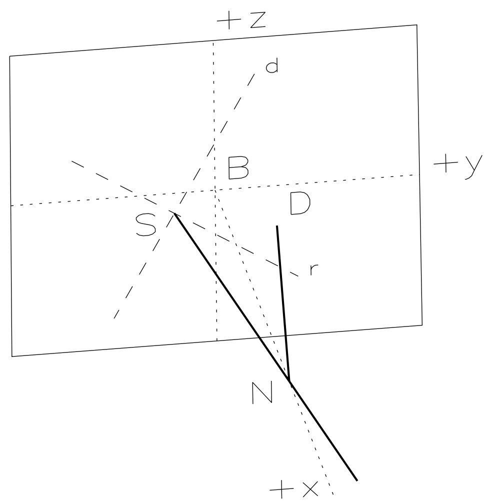

Figure 2: *This figure shows a schematic perspective view of a beam from the HRMA diffracting at the grating node, N, into the direct beam to point S, and the diffracted beam to point D. The focal-plane coordinates are (y, z), whose axes are marked by dotted lines; $+y$ is the approximate positive order diffraction direction while z is the Science Instrument Module translation direction. The grating coordinates are defined by the direction of dispersion and are marked by the dashed lines. D is not necessarily on the dispersion line due to scattering and aberrations. The detector surface follows the Rowland circle which is concave toward the HRMA (but the curvature is not shown in this diagram). The aim-point (bore-sight) is at B. NB is nominally normal to the facet.*

$\vec{S}$ is the vector from the node, N, to the source position, S.

$\vec{D}$ is the vector from the node, N, to the diffracted photon position, D.

$\hat{x}$ is the unit vector in the AXAF focal plane coordinate system plus x direction, which is directed *from the node, N, towards the HRMA.*

$\hat{y}$ is the focal-plane y direction unit vector.

$\hat{z}$ is the focal-plane z direction unit vector.

$\hat{r}$ is the unit vector in the positive order dispersion direction. For $\alpha = 0$, this is parallel to $\hat{y}$.

$\hat{d}$ is the unit vector in the cross-dispersion direction. For $\alpha = 0$, this is parallel to $\hat{z}$.

X_{R} is the Rowland diameter (8635 mm), the designed length of NB. Since the spectroscopic detectors are tiled to follow the Rowland circle, any point on the detector is never far from X_{R} (in particular, $|\vec{S}|$ is very nearly equal to X_{R}).

The coordinate systems defined by $(\hat{x}, \hat{y}, \hat{z})$ and by $(\hat{x}, \hat{r}, \hat{d})$ are both cartesian orthonormal systems. I assume that D, S, and N are known in three-dimensional spatial (x, y, z) coordinates in the focal plane, and that α is known relative to y. I also assume that N is on the HRMA axis.

For a detailed description of AXAF coordinate systems and their transformations, see "ASC Coordinates: Rev 2.3 Draft", J. McDowell, January 9, 1996, or a later revision.)

2.2 Transformation of Coordinates

The primary goal is to determine the most probable wavelength of the photon retiring from its long journey at D. In general this is a convolution problem involving the probability distribution functions of the combined optical elements ("point spread functions") and the source spectral distribution. If D is not in the r-direction from S, its most probable wavelength (under simple diffraction theory) is that wavelength of the nearest point on the Rowland circle (i.e., the perpendicular projection onto r).

Here, I intend to derive one parameter which is to first order proportional to the wavelength, and a second parameter which can be used for further refinements, if desired. These quantities are the angular deviations in the dispersion direction, θ_r, and in the cross-dispersion direction, θ_d. We can then use the dispersion relation in its simplest form to determine the wavelength:

$$m\lambda = P \sin\theta_r,$$

where m is the diffraction order (an integer), λ is the photon wavelength, and P is the average grating period.

For the full 3-D formulation of this relevant to higher order terms, see ASC memo by J. Davis (in draft form, as of 2/22/96).

We actually can only determine the product, $m\lambda$, unless we have additional information.

2.2.1 Transformation and Projection

To determine the diffraction angle, we must project $\vec{D}$ onto the r-direction $(\vec{D} \cdot \hat{r})$. That length – at some distance from N – defines the diffraction angle. For that distance, we choose the component of $\vec{D}$ in the direction of $\vec{S}$, D_S.

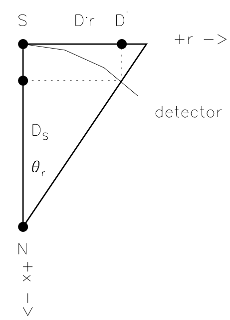

Figure 3: *The projection of $\vec{D}$ onto the $\hat{r}$ direction is shown in the plane defined by $\vec{S}$ and $\hat{r}$. The point, D', is the endpoint of the projection of $\vec{D}$ onto r. The curved line represents the detector in cross-section following the Rowland torus. The length, $\vec{D}\cdot\hat{r}$, at the distance of D_S defines the angle, θ_r, as described in the text.*

We first relate the orthonormal r, d coordinates to the orthonormal x, y, z system via a rotation of coordinates by the diffraction "clocking" angle, α:

$$\hat{r} = 0\,\hat{i} + \cos\alpha\,\hat{j} + \sin\alpha\,\hat{k},$$

and

$$\hat{d} = 0\,\hat{i} - \sin\alpha\,\hat{j} + \cos\alpha\,\hat{k}.$$

The component of $\vec{D}$ in the direction of $\vec{S}$ is

$$D_S = \frac{\vec{D}\cdot\vec{S}}{|\vec{S}|} = \frac{D_x S_x + D_y S_y + D_z S_z}{\sqrt{S_x^2 + S_y^2 + S_z^2}}.$$

The angles are simply expressed in terms of their tangents, which is also convenient and unambiguous because the angles are small:

$$\tan\theta_r = \frac{\vec{D}\cdot\hat{r}}{D_S} = (D_y\cos\alpha + D_z\sin\alpha)/D_S.$$

Figure 3 shows the relevant geometry in the $\hat{r} - \hat{S}$-plane.

We can analogously solve for θ_d:

$$\tan\theta_d = \frac{\vec{D}\cdot\hat{d}}{D_S} = (-D_y\sin\alpha + D_z\cos\alpha)/D_S.$$

These then define the necessary angles for determining the photon's grating nodal coordinates. It should be noted that the source position is a necessary quantity in this transformation. If there are multiple sources in a field, then there will necessarily be multiple transformations, and regions for which coordinates are ambiguous, depending on which source the photons are attributed to.

2.2.2 Coordinate Scaling

It is convenient to scale the angles to some fiducial configuration. A logical choice is millimeters at the Rowland diameter. Observations with slightly different pointings or defocus would then have identical scales, but different blur properties. Thus we define the penultimate diffraction grating nodal coordinates, $r_{\mathrm{T}G}$ and $d_{\mathrm{T}G}$, the dispersion and cross-dispersion coordinates:

$$r_{\mathrm{T}G} = X_{\mathrm{R}}\theta_r, \quad d_{\mathrm{T}G} = X_{\mathrm{R}} \tan\theta_d.$$

The former is expressed as an arc length, since the detectors approximately tile the Rowland circle in the r-dimension. The other has been projected into a line, since the detectors are linear in the z-dimension.

2.2.3 A Simplified Case

For a simplified example, let $\alpha = 0$ and $S = (X_{\mathrm{R}}, 0, 0)$. This is like LETG with the source at the aim-point. Then we find that $\tan\theta_r = D_y/D_x$, and $\tan\theta_d = D_z/D_x$, as expected.

2.2.4 Tabular Data

Table 1: Parameters of the HETG and LETG Spectrometers

Grating	Period [Å]	α [deg]	Scale [Å/mm]
HEG	2000	-5	0.232
MEG	4000	+5	0.463
LEG	9921	0	1.149

3 Simplifying Conditions

Since the Rowland diameter is large compared to the length of the spectroscopic arrays, it is a good approximation that $D_x \approx S_x$. And since the arrays closely tile the Rowland circle, the linear distance along the arrays (a "segmented" coordinate) is essentially the arc-length along the Rowland circle. Hence,

$$\theta_r \approx (D_y \cos\alpha + D_z \sin\alpha)/S_x.$$

The distance, S_x, could be slightly different from the Rowland diameter by any defocus: $S_x = X_{\mathrm{R}} + \epsilon$, where ϵ is on the order of a few tenths of a millimeter.

In the cross-dispersion direction, we can also use $D_x \approx S_x$, but since the detector is flat in that direction, we use

$$\theta_d \approx \arctan\left(-D_y \sin\alpha + D_z \cos\alpha\right)/S_x.$$

Figure 4 shows the deviations from ideal if linear pixel distances along the detector are used instead of the exact conversion into angle. The HRC-S configuration is the largest deviation expected since the HRC-S segments are longer than ACIS-S and deviate most from the Rowland Circle. The errors incurred are less than one HRC pixel, which is itself about one-quarter of a resolution elements.

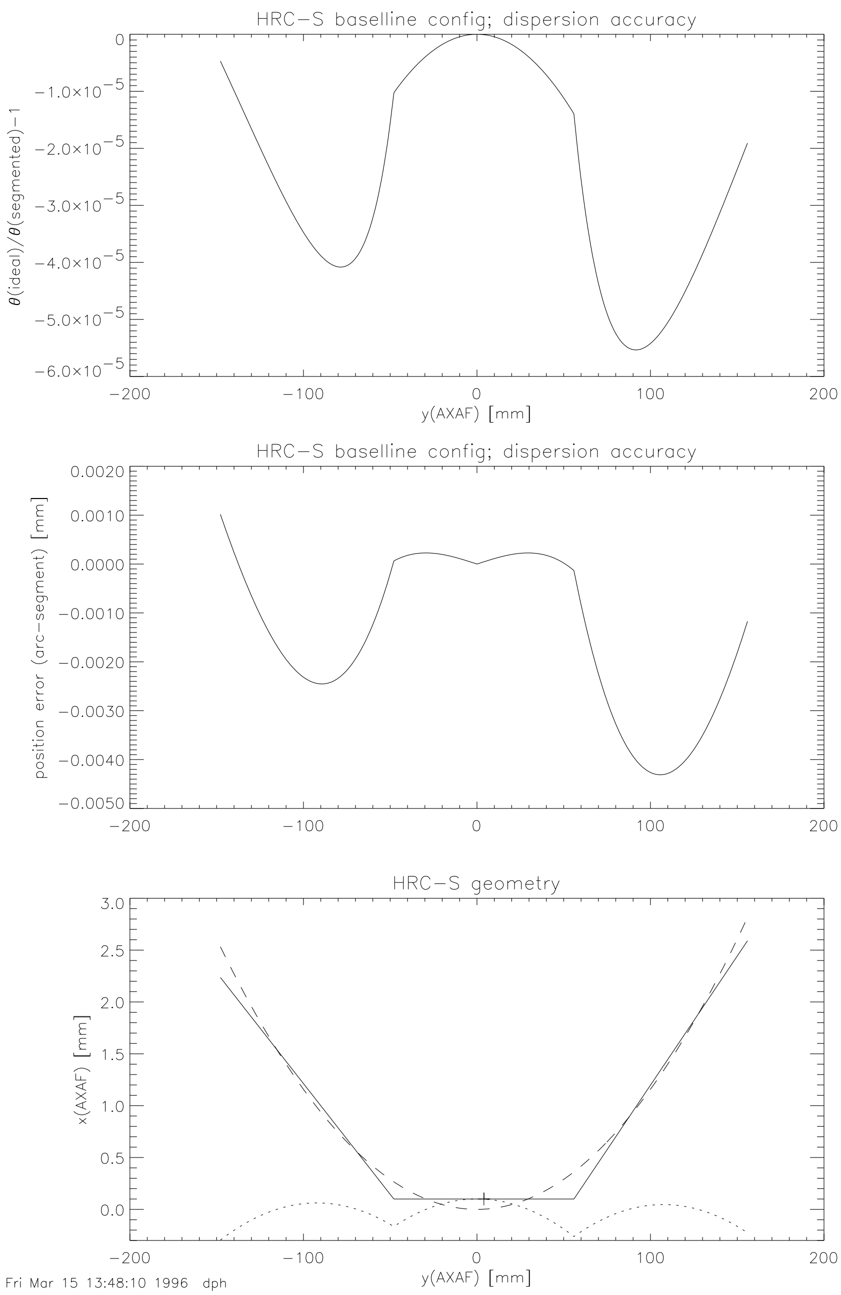

Figure 4: *If the linear distance along HRC-S segments – which deviate most, compared to ACIS-S, from the Rowland circle – are used to approximate the Rowland circle arc-length, errors are negligible. The top panel shows the fractional deviation from the ideal angle. The middle panel shows the linear error incurred by this angle at the Rowland diameter distance; one HRC pixel is 0.0064 μm. These two curves are for a source at the aim-point at the nominal focus. The bottom panel shows the relative geometries of the HRC-S segments (solid lines) and the Rowland circle (dashed line); the dotted line shows their difference.*