Coordinate Systems for Analysis of On-Orbit Chandra Data
Paper III: Dispersed Spectra

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1 Introduction

The Chandra X-ray Observatory, launched in July 1999, provides X-ray imaging and spectral data of unprecedented resolution. The geometry of Chandra's detectors is more complicated than those of previous missions; this, coupled with the higher accuracy requirements, means that more care must be taken to derive accurate coordinates and to distinguish clearly between different coordinate systems.

In the first two papers in this series we discussed calculation of image space coordinates. In the present note, we consider interpretation of grating data.

1.1 Chandra gratings

The Chandra X-ray Observatory has two transmission gratings, the HETG (High Energy Transmission Grating) and the LETG (Low Energy Transmission Grating). Each of these is physically a large circular structure consisting of four annuli matched to the radii of the four HRMA (High Resolution Mirror Array) mirror pairs. Around the annuli are mounted hundreds of individual grating facets. The grating structures are attached to the back of the HRMA with hinges so that either of them may be rotated around to intercept the rays emerging from the mirrors. The LETG facets, collectively the LEG (Low Energy Grating), have a period of around 9900Å and are aligned so that the light is dispersed along the telescope FCY (paper I) axis, perpendicular to the direction of optical bench motion and aligned with the long direction of the HRC-S and ACIS-S detectors. The HETG has two sets of facets, known as HEG (High Energy Grating) and MEG (Medium Energy Grating), with periods of 2000 and 4000Å respectively. The HEG and MEG dispersion directions are each inclined about 5 degrees to the FCY axis so that the dispersed spectra form an X shape on the imaging detectors. In normal use, the LETG is employed in conjunction with the HRC-S detector, since ACIS doesn't have good response at low energy. The HETG is employed with the ACIS-S detector, whose independent CCD energy resolution facilitates order separation.

In the idealization we adopt here, light from the HRMA passes through a single point G, the grating node, from which it is dispersed by an angle θ along the grating dispersion direction. We refer to the LEG, HEG and MEG as 'grating arms' and consider only one grating arm at a time.

The distance between G and the focus F is the Rowland distance R, and the best focus for the dispersed photons lies along a circle in the dispersion plane centered on G with radius R.

A photon of wavelength λ passing through G will be deflected by an angle

$$r = \sin^{-1}(m\lambda/P)$$

where P is the 'grating period' and m, an integer, is the 'order'. Most photons enter the zero order spectrum with m=0, and land exactly where they would have if the grating had not been present - the zero order position ZO. The next most probable fate for the photons is to be deflected into the m=1 or m=-1 first order spectra; successively higher order spectra contain less and less of the total incident energy.

2 Source based coordinate systems

To analyse the geometry of a spectrum we need to set up coordinate systems for a particular source. Note that if multiple sources are present in the field, their spectra will overlap on the detector making analysis difficult.

Consider a sphere whose equatorial plane lies in the dispersion direction and whose center is at $\boldsymbol{G}$. Then the dispersion angle r is just longitude on the sphere relative to a meridian passing through the line $\boldsymbol{S}$ joining $\boldsymbol{G}$ with $\boldsymbol{ZO}$, the source's zero order position. The latitude d is called the cross-dispersion angle.

If the source is on axis, $\boldsymbol{ZO}$ lies at the imaging aimpoint and in the mirror nodal coordinates of paper I the pole of the sphere has coordinates

$$\boldsymbol{d_0} = (0, -\sin\alpha_G, \cos\alpha_G) \tag{1}$$

where α_G is the angle between the dispersion direction and the spacecraft Y axis. For an off-axis source, the dispersion direction is perpendicular to both $\boldsymbol{d_0}$ and $\boldsymbol{S}$; we define a cartesian orthonormal set of Grating Zero Order coordinates (GZO)

$$\begin{aligned} \boldsymbol{e}_{X_{ZO}} &= -\boldsymbol{S}/|\boldsymbol{S}| \\ \boldsymbol{e}_{Y_{ZO}} &= \boldsymbol{d_0} \wedge \boldsymbol{e}_{X_{ZO}}/|\boldsymbol{d_0} \wedge \boldsymbol{e}_{X_{ZO}}| \\ \boldsymbol{e}_{Z_{ZO}} &= \boldsymbol{e}_{X_{ZO}} \wedge \boldsymbol{e}_{Y_{ZO}} \end{aligned} \tag{2}$$

with origin at G. Diffracted photons travel in the X_{ZO}, Y_{ZO} plane, and the intersection of this plane with the detector surface defines the dispersion direction.

To calculate the wavelength of a photon, we go through several steps:

1. We use the equations of paper I to convert from detected chip coordinates to focal coordinates (FCX,FCY,FCZ), correcting for the chip position on the SIM and for the SIM translation and boresight. We now have the position of the dispersed photon relative to the mirror axis (assumed to coincide with the grating axis).

2. We then calculate the GZO coordinates of the photon by subtracting the FC coordinates of G (which are just (R,0,0)) and applying a rotation matrix to account for the misalignment of the GZO axes with the FC axes.

$$\begin{pmatrix} X_{GZO} \\ Y_{GZO} \\ Z_{GZO} \end{pmatrix} = R(FC, GZO) \left(\begin{pmatrix} X_{FC} \\ Y_{FC} \\ Z_{FC} \end{pmatrix} - \begin{pmatrix} R \\ 0 \\ 0 \end{pmatrix} \right)$$

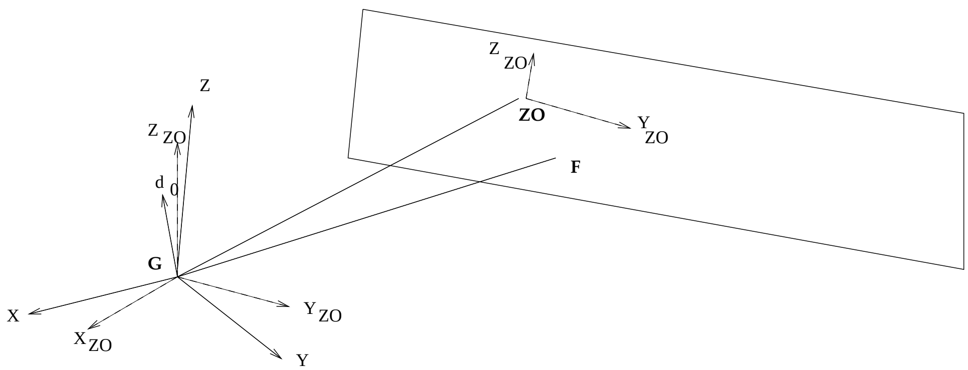

Figure 1: Grating Zero Order coordinates

3. We now convert from GZO coordinates to longitude and latitude on the GZO sphere,

$$
\begin{aligned}
r &= \tan^{-1}\left(\frac{-Y_{GZO}}{X_{GZO}}\right) && \sim -Y_{GZO}/X_{GZO} \\
d &= \tan^{-1}\left(\frac{+Z_{GZO}}{\sqrt{X_{GZO}^2+Y_{GZO}^2}}\right) && \sim +Z_{GZO}/X_{GZO}
\end{aligned} \tag{3}
$$

4. Finally, we apply the dispersion relation

$$\lambda = P \sin r/m$$

to derive the wavelength assuming the order m is known.

2.1 Grating Diffraction Plane Pixel Coordinates (GDP-1.1)

For analysis purposes it may be useful to define a standard pixel system for creating grating images. The Grating Diffraction Plane Pixel Coordinates GDX, GDY are defined by

$$
\begin{aligned}
GDX &= GDX0 - \Delta_{gs}^{-1}(Y_{ZO}/X_{ZO}) \\
GDY &= GDY0 + \Delta_{gs}^{-1}(Z_{ZO}/X_{ZO})
\end{aligned} \tag{4}
$$

analogously to the Focal Plane Pixel Coordinates. The pixel size Δ_{gs} is chosen to match the instrument physical pixel size (and in the current GDP-1.1 system is set to 0.154 arcsec, with GDX0 = GDY0 = 32768.50 pixels).

They are related to the angular Grating Diffraction Coordinates by

$$
\begin{aligned}
GDX &= GDX0 + \Delta_{gs}^{-1} \tan r \\
GDY &= GDY0 + \Delta_{gs}^{-1} \tan d \cos r
\end{aligned} \tag{5}
$$

3 In-flight numerical values for Chandra

The Rowland diameter is 8632.48mm.

Table 1: Grating properties

Instrument	P	α_G (deg)

HETG	2000.81Å	-5.18
METG	4001.41Å	4.75
LETG	9912.16Å	+0.016

4 Summary

In this paper we summarized the calculations used by the Chandra data processing system to assign wavelengths to photons in transmission grating data. The formalism is sufficiently general that it should be applicable to other missions by appropriately changing the numerical values in section 3.

We thank Dave Huenemorder and Dan Dewey for useful discussions, and Helen He for implementing the software routines used to apply the coordinate transforms in the Chandra data processing system.

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